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VICE PRESIDENT
CHEMSTAR

American Chemistry Council Good Chemistry Makes It Possible

201-14980

December 29, 2003

Via Messenger and CD-Rom

Michael O. Leavitt, Administrator
U.S. Environmental Protection Agency
P.O. Box 1473
Merrifield, VA 22116

Re: Fatty Nitrogen Derivatives Panel Nitriles Task Group, Consortium No. HPV Chemical Challenge Program Submission of Nitriles Category Justification and Testing Rationale

Dear Administrator Leavitt:

The Fatty Nitrogen Derivatives Panel Nitriles Task Group of the American Chemistry Council submits the subject documents to EPA's HPV Chemical Challenge Program as its test plan for a category covering 14 chemicals. The Nitriles Task Group includes the following member companies that are sponsoring these chemicals under the Voluntary HPV Chemical Challenge Program: Akzo Nobel Chemicals Inc.; Crompton Corporation; and Goldschmidt Chemical Corporation.

This submission includes the following documents:

- Fatty Nitrogen Derived Nitriles Category High Production Volume (HPV) Chemical Challenge – Assessment of Data Availability and Test Plan and
- Appendix A: Robust Summaries for Reliable Studies.

Due to the size of the files, this submission is also being sent via CD-Rom to the above address. An email will be sent to the following email addresses to notify EPA of the submission:

Oppt.ncic@epa.gov
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If you require additional information, please contact F. J. "Sonny" Maher, Fatty Nitrogen Derivatives Panel Manager at (703) 741-5605 or sonny_maher@americanchemistry.com.

Sincerely yours,

Courtney M. Price
Vice President, CHEMSTAR

Attachment
cc: Nitriles Task Group
Steve Russell, ACC
Jim Keith, ACC

201-14980

Fatty Nitrogen Derived Nitriles Category High Production Volume (HPV) Chemicals Challenge Program

Assessment of Data Availability and Test Plan

Prepared for:

American Chemistry Council
Fatty Nitrogen Derivatives Panel
Nitriles Task Group

Prepared by:

Toxicology/Regulatory Services, Inc.

December 29, 2003

Fatty Nitrogen Derived Nitriles Category
High Production Volume (HPV) Chemicals Challenge Program
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Introduction

The Fatty Nitrogen Derived (FND) Nitriles Category chemicals are closed-system intermediates that fall within the realm of the U.S. EPA HPV Chemicals Challenge Program. This category includes 14 FND Nitriles chemicals that are similar as to their physical/chemical properties, environmental fate, ecotoxicity, and human health-related data. The chemicals in this category have been evaluated according to the EPA "Guidance for Testing Closed System Intermediates for the HPV Challenge Program" (U.S. EPA, 1999a). The potential for exposure to the chemicals is a key component of the determination of data development needs for the chemical category, under the HPV Program.

In the following paragraphs, on behalf of the member companies, the American Chemistry Council (ACC) FND Panel Nitriles Task Group (Task Group) provides information which substantiates the position that the FND Nitriles Category chemicals, produced at manufacturing facilities of member companies, meet the definition of closed-system intermediates in the context of the EPA HPV Chemicals Challenge Program.

By definition, closed-system intermediates have a limited potential for release to the environment. In the Challenge Program there are two types of intermediates that are contained in "closed system":

a) Isolated intermediates that are stored in controlled on-site facilities; and
b) Isolated intermediates with controlled transport, i.e. to a limited number of locations within the same company or second parties, which use the chemical in a controlled way as an intermediate with well-known technology.

The companies represented in the ACC FND Panel Nitriles Task Group are major producers of FND Nitriles Category chemicals in the United States. The FND Nitriles Category chemicals sponsored by the ACC FND Panel Nitriles Task Group member companies are eligible for the closed-system intermediates provisions because they fulfill criterion a or b or both in the above definition, as discussed below

The table below shows that FND Nitriles Category chemicals also meet the definition for limited exposure potential based on the limited number of manufacturing sites handling these chemicals. These sites can be either production sites for FND Nitriles Category chemical intermediates or sites where the FND Nitriles Category chemicals are further derivatized.

Number of US Manufacturing Sites for FND Nitrile Category Chemicals

	Akzo Nobel	**Goldschmidt**	**Crompton**
Total Number of Sites	5	1	1
Company Sites:			
▪ In the U.S.	2	1	1
▪ Outside the U.S.	3		
Second Party Sites	0	0	0

FND Nitriles Category chemicals are used as intermediates and their use occurs in closed systems. Little to no exposure to workers is expected because the reaction vessels used to manufacture FND Nitriles Category chemicals are part of multi-purpose, closed-system operations. Generally, the equipment is cleaned only after production campaigns, which occur several times per year. Wastewater generated during routine maintenance of the process equipment (occurring typically twice per year) and storage tanks at the Task Group member company facilities is disposed of subject to requirements set forth in current state and federal environmental regulations. Site wastewater is routed to on-site treatment systems where the trace amounts of chemicals present undergo further dilution and microbial degradation, or wastewater is routed directly to an on-site incinerator where it is used as a fuel in the incinerator. These systems help limit environmental releases.

Monitoring data are not routinely collected to assess for potential exposures to FND Nitriles Category chemicals. However, as the toxicological summary contained in this assessment report demonstrates, all of the chemicals in the FND Nitriles Category have a low order of acute toxicity and are not mutagenic.

Routine chemical analyses are not typically conducted for trace amounts of unreacted FND Nitriles Category chemicals in downstream derivatives, but the economics of chemical production drive complete reaction of the intermediate chemicals. Furthermore, the efficiency of conversion to primary amines, the next derivative in the manufacturing process, is typically greater than 99%. Levels of unreacted FND Nitriles Category chemicals in downstream derivatives are also minimized because the odor associated with even trace amounts of FND Nitriles Category chemicals is regarded as unpleasant and can be problematic in downstream products.

As mentioned previously, FND Nitriles Category chemicals can be manufactured at one site and derivatized at a different site. Transportation typically is made in tank truck and tank car to the other company sites. Transfer from storage tanks to transport vehicles and then to either storage tanks or reaction vessels at other company sites is a controlled and routine operation. Should a line or pump fail during one of these operations, all sites use typical spill containment methods to help minimize any environmental contamination. In the unlikely event of an accidental spill or release during transit between locations, FND Nitriles Category chemicals have been shown to be inherently or readily biodegradable in studies conducted under Organization for Economic Cooperation and Development (OECD) test guidelines.

The limited environmental and human exposure potential during production, limited release potential during transportation, and data showing the chemicals' low order of acute toxicity and lack of mutagenicity substantiate the Task Group's decision to follow the reduced testing plan as described in the "Guidance for Testing Closed System Intermediates for the HPV Challenge Program" (U.S. EPA, 1999a). Testing beyond that for the closed-system intermediates is not warranted.

Definition of Fatty Nitrogen Derived (FND) Nitriles Structure-Based Chemical Category

The FND Nitriles Category is comprised of 14 separate chemicals with unique CAS Registry Numbers (RNs). The FND Nitriles Category chemicals are identified in the following table:

Table A: CAS Registry Numbers and Chemical Names

CAS RN	Chemical Name
112-91-4	9-Octadecanenitrile
629-79-8	Hexadecanenitrile
638-65-3	Octadecanenitrile
2437-25-4	Dodecanenitrile
26351-32-6	Propanenitrile, 3-(9-Octadecenylamino)-, (Z)-
61789-53-5	Nitriles, coco
61790-28-1	Nitriles, tallow
61790-29-2	Nitriles, tallow, hydrogenated
68002-64-2	Nitriles, C16 and C18 unsaturated
68002-65-3	Nitriles, C16-18
68153-02-6	Nitriles, C16-22
68513-04-2	Nitriles, C14-18 and C16-18 unsaturated
68514-67-0	Nitriles, soya
68784-70-3	Propanenitrile, 3-amino-, N-tallow alkyl derivatives

Structural Information for the FND Nitriles Category

The following table presents the molecular formula and molecular weight data for the FND Nitriles Category chemicals with defined structures or structures for which average chain lengths can be determined. The structures for these and the remaining chemicals in the category are provided in Table 1.

Table B: Molecular Formula and Molecular Weight of Chemicals with Defined Structures

CAS RN	Chemical Name	Molecular Formula	Molecular Weight
2437-25-4	Dodecanenitrile	$C_{12}H_{23}N$	181
629-79-8	Hexadecanenitrile	$C_{16}H_{31}N$	237
638-65-3	Octadecanenitrile	$C_{18}H_{35}N$	265
68002-65-	Nitriles, C16-18	$C_{17}H_{33}N$	251[a]

3			
68153-02-6	Nitriles, C16-22	$C_{19}H_{37}N$	279[b]
112-91-4	9-Octadecenenitrile	$C_{18}H_{33}N$	263
26351-32-6	Propanenitrile, 3-(9-Octadecenylamino)-, (Z)-	$C_{21}H_{40}N_2$	320

[a] Based on average chain length = 17
[b] Based on average chain length = 19

Rationale for the FND Nitriles Structure-Based Chemical Category

The members of the FND Nitriles category are large molecules. The structure of these molecules result in surfactant-like properties that have physical/chemical properties, environmental fate, and toxicity similar to an even larger family of surfactants including the FND amines, cationics, and amides (each submitted as a separate category in the HPV Chemical Challenge Program). The following table summarizes the long-chain alkyl substituents found in the FND Nitriles Category Chemicals:

Table C: Chain Length and Degree of Unsaturation for Long-Chain Substituents in the FND Nitriles Category Chemicals

Identifier	Chain Length(s) or Average	Degree of Unsaturation
Dodecane	12	None
Hexadecane	16	None
Octadecane	18	None
C16-C18	Not specified	None
C16-C22	Not specified	None
C14-C18 and C16-C18-unsaturated	Not specified	Not specified
C16 and C18-unsaturated	Not specified	Not specified
Octadecene	18	1
Octadecenyl	18	1
Coco (coconut)	C6: 0-1% C8: 5-9% C10: 5-10% C12: 44-53% C14: 13-19% C16: 8-11% C18: 1-3% C16: 0-1% C18: 5-8% C18: 1-3%	None None None None None None None 1 1 2
Tallow, hydrogenated[1]	C14: 1-6% C16: 23-46% C18: 49-67%	None None None
Tallow	C14: 1-6%	None

[1] Percentages assume 100% hydrogenation of the unsaturated tallow chains.

Table C: Chain Length and Degree of Unsaturation for Long-Chain Substituents in the FND Nitriles Category Chemicals

Identifier	Chain Length(s) or Average	Degree of Unsaturation
	C16: 20-37% C18: 14-21% C16: 3-9% C18: 35-46% C18: 4-10% C18: 0-3%	None None 1 1 2 3
Soya (soy bean)	C16: 7-11% C18: 2-7% C20: 0-2% C18: 20-30% C18: 43-56% C18: 8-14%	None None None 1 2 3

As noted in the table above, the fatty acids used for production of the FND Nitriles Category Chemicals are all similar in composition. Overall, the chain length and degree of unsaturation in the FND chemicals have little impact on fate and effects. These chemicals, by the nature of their surfactant properties, are toxic to aquatic organisms at low concentrations. A careful examination of the chemical structures (Table 1) shows a close relationship among all of the chemicals in the category. The following discussion highlights the structural similarities.

Dodecanenitrile, hexadecanenitrile and octadecanenitrile are fixed chain-length substituted nitriles of 12, 16, and 18 carbons, respectively. The available data shows that, over this range, the FND Nitrile Category chemicals as well as the other FND chemicals (amines, cationics, amides) are not expected to, nor exhibit, significant differences in the HPV/SIDS endpoints. Therefore, for the purposes of this screening program, these chemicals are considered essentially equivalent. The remaining alkane-substituted nitriles and 3-aminopropane nitriles have carbon chain distributions ranging from C14 to C22. Several of these chemicals contain minimally unsaturated alkyl chains. Across the FND chemicals, available data show that the degree of unsaturation of the alkyl chain does not alter the toxicological properties of these chemicals. Overall, tallow and hydrogenated tallow are considered identical. Since the natural oils from coconut and soybean are similar to the tallow oils, varying only in percent of chain lengths and degree of unsaturation, all of the natural oil substituted nitriles are essentially the same. These natural oils are also similar to the defined chain length alkyl substituents. Thus, considering the structural similarities and consistent toxicological properties, there are no significant differences among the chemicals in the category that reasonably can be expected to result in differences in the HPV/SIDS endpoints.

Available Data to Fulfill HPV Screening Information Data Set (SIDS) Endpoints

Approach to Evaluate the Database for the FND Nitriles Category

Special approaches related to closed-system intermediates: Closed-system intermediates are evaluated differently from other HPV chemicals (U. S. EPA, 1999a). The guidance document specifies that "*exposure considerations can impact the battery of tests performed…*". Further, EPA provides the following guidance: *"For closed system intermediates a reduced test plan package reflecting the information needed to evaluate the hazards in case of an accident is considered the appropriate level of testing for screening purposes. This is because exposures resulting from chemical accidents are likely to be of relatively short versus chronic duration. The reduced testing consists of the Screening Information Data Set (SIDS) minus the tests for repeated dose toxicity and reproductive toxicity, but including a developmental toxicity test."*

The following approach was used to obtain and analyze data relevant to the assessment of the FND Nitriles Category chemicals.

1. The chemical names and CAS RNs of the 14 HPV FND Nitriles Category chemicals supported by the Task Group were provided.
2. As available, published and unpublished reports were obtained from the members of the Task Group and other sources; they were organized and reviewed to identify studies that could fulfill SIDS endpoints.
3. Pertinent publicly available databases[2] were searched and all identified relevant reports were obtained to establish the full extent and nature of the published literature for the 14 HPV FND Nitriles Category chemicals.
4. Each of the reports obtained was reviewed to determine its adequacy for use in the EPA HPV Chemicals Challenge Program according to EPA criteria and reliability scoring according to Klimisch *et al.* (1997).
5. Robust Summaries were prepared for each report with a Klimisch score of 1 or 2, according to the guidelines proposed by the EPA (U.S. EPA, 1999b) for each study type.
6. Estimates were developed for physical/chemical properties and environmental fate and ecotoxicity endpoints by using appropriate Structure Activity Relationships (SARs).
7. Fugacity modeling (Level 3) was performed to estimate transport and distribution into environmental compartments for the FND Nitriles Category chemicals.

[2] Databases include ChemIDplus, HSDB (Hazardous Substances Data Bank), IRIS (Integrated Risk Information System), CCRIS (Chemical Carcinogenesis Research Information System), GENE-TOX, EMIC (Environmental Mutagen Information Center), DART/ETIC (Developmental and Reproductive Toxicology and Environmental Teratology Information Center), MEDLINE, TOXLINE, RTECS (Registry of Toxic Effects of Chemical Substances),TSCATS (Toxic Substances Control Act Test Submissions), IUCLID (International Uniform Chemical Information Database), 1996.

Use of Structure-Activity Relationships for the FND Nitriles Category

Approaches recommended in the EPA document on the use of SARs in the EPA HPV Chemicals Challenge Program were employed in the assessment of the FND Nitriles Category chemicals (U.S. EPA, 1999c). Several models were employed to support the review and assessment of the FND Nitriles Category chemicals. The models included several SARs, as well as Mackay-type fugacity-based modeling. The SAR models for physical properties were used to estimate boiling point, melting point, aqueous solubility, octanol-water partition coefficient and vapor pressure. Other SAR models were used to estimate hydroxyl radical mediated atmospheric photo-oxidation and biodegradation potential. SAR models also were used to obtain estimates of acute toxicity to aquatic organisms.

Common Features of the Models

All of the models (except the Mackay-type models) require the input of a molecular structure to perform the calculations. The structure must be entered into the model in the form of a SMILES (Simplified Molecular Input Line Entry System) notation or string. SMILES is a chemical notation system used to represent a molecular structure by a linear string of symbols. The SMILES string allows the program to identify the presence or absence of structural features used by the submodels to determine the specific endpoint. The models contain files of structures and SMILES strings for approximately 100,000 compounds, accessible via CAS RNs. SMILES strings cannot be developed for mixtures or chemicals without a single, definable structure.

Estimation of Physical/Chemical Properties

The SAR models for estimating physical properties and abiotic degradation were obtained from Syracuse Research Corporation 2000 (Estimation Programs Interface for Windows, Version 3.05 or EPIWIN v.3.10). The models were used to calculate melting point, boiling point, vapor pressure (submodel MPBPVP), octanol-water partition coefficient (K_{ow}) (submodel KOWWIN), and aqueous solubility (submodel WSKOWWIN). The calculation procedures are described in the program guidance and are adapted from standard procedures based on analysis of key structural features (Meylan and Howard, 1999a, b, and c).

Estimation of Environmental Fate Properties

Atmospheric photo-oxidation potential was estimated using the submodel AOPWIN (Meylan and Howard, 2000). The estimation methods employed by AOPWIN are based on the SAR methods developed by Dr. Roger Atkinson and co-workers (Meylan and Howard, 2000). The SAR methods rely on structural features of the subject chemical. The model calculates a second-order rate constant with units of cm^3/molecules-sec. Photodegradation based on atmospheric photo-oxidation is in turn based on the rate of reaction (cm^3/molecules-sec) with hydroxyl radicals (HO•), assuming first-order kinetics and an HO• concentration of 1.5^6 molecules/cm^3 and 12 hours of daylight. Pseudo first-order half-lives ($t_{1/2}$) were then calculated as follows: $t_{1/2} = 0.693/[(k_{phot} \times HO\bullet) \times (12\text{-hr}/24\text{-hr})]$.

The HYDROWIN database that supports the modeling of water stability provides only for neutral organic compounds that have structures that can be hydrolyzed. Therefore, no model

estimates for hydrolytic stability are available since the FND Nitriles Category chemicals do not have the necessary characteristics.

Estimation of Environmental Distribution

The Level 3 Mackay-type, fugacity based models were obtained from the Trent University's Modeling Center. The specific model used was the generic Equilibrium Concentration model (EQC) Level 3, version 1.01. These models are described in Mackay *et al*. (1996a and b). Fugacity-based modeling is based on the "escaping" tendencies of chemicals from one phase to another. For instance, a Henry's Law constant calculated from aqueous solubility and vapor pressure is used to describe the "escape" of a chemical from water to air or vice versa as equilibrium between the phases is attained. Key physical properties required as input parameters into the model are melting point, vapor pressure, K_{ow} and aqueous solubility. The model also requires estimates of first-order half-lives in the air, water, soil, and sediment. An additional key input parameter is initial loading of the chemical into the environment.

Estimation of Acute Aquatic Toxicity

Models developed by the U.S. Environmental Protection Agency (EPA) were employed to make estimates of acute toxicity to aquatic organisms, specifically a commonly tested fish, the fathead minnow (*Pimephales promelas*), a water column dwelling invertebrate, *Daphnia magna*, and a commonly tested green alga, *Selenastrum capricornutum*. The models are incorporated in a modeling package called ECOSAR, version 0.99g (U. S. EPA, 2000). ECOSAR may be obtained from the EPA website for the Office of Pollution Prevention and Toxics, Risk Assessment Division. The models calculate toxicity based on structural features and physical properties, mainly the K_{ow} (Meylan and Howard, 1998).

Modeling Information Specific for FND Nitriles Category Chemicals

Where possible, the models described above were used for the FND Nitriles Category chemicals. Estimations of physical properties, environmental fate and distribution, and ecotoxicity were not possible for 7 of the 14 HPV chemicals in the FND Nitriles Category because they do not have single definable structures. The model did not provide estimates of stability in water for this class of chemicals because the model cannot calculate this parameter for chemicals that do not meet the criteria of neutral organic compounds with structures that can be hydrolyzed. However, since the FND Nitriles Category chemicals are closed-system intermediates, direct release of these chemicals into the environment is not expected under normal operating conditions. To provide a means of fugacity modeling, all input was assumed to be into surface water, representing the "worst-case" scenario for an accidental release, using the chemical- specific parameters to attain estimates of the chemical distributions between environmental compartments.

Physical/Chemical Properties Reliable Data and SAR Estimates

The available reliable data and SAR estimates for physical/chemical properties of the FND Nitriles Category chemicals are presented in Table 2. Robust Summaries for the reliable studies

and SAR estimates are provided in Appendix A. The Test Plan for Physical/Chemical Properties is outlined in Table 4.

Measured data for melting points for the FND Nitriles Category chemicals ranged from < -22 to 41°C. The modeled values ranged from 25 to 148°C. Measured data for boiling points ranged from 220 to 390°C. The modeled boiling point values ranged from 277 to 418°C.

Consistent with similar, large organic molecules, the measured and EPIWIN estimated vapor pressures were low (even at temperatures as high as 200°C) across the FND Nitriles Category, with all values ≤ 0.002 mm Hg for the measured and modeled data, respectively.

The measured and EPIWIN estimated values for the octanol/water partition coefficient (log K_{ow}) ranged from 4.9 to > 6 and 6.1 to 8.2, respectively.

Measured values and model predictions for water solubility indicated that the FND Nitriles Category chemicals have very limited solubility or are insoluble. Reported data indicated that these chemicals are 'insoluble' or 'practically insoluble' and model estimates ranged from 0.0009 to 1.9 mg/l.

Summary – Physical/Chemical Properties

Overall, the FND Nitriles Category chemicals have relatively low melting points when measured or modeled (generally < 100°C) and moderate boiling points, showing chemical decomposition in one case when measured (9-octadecenenitrile). The FND Nitriles Category chemicals are nonvolatile. The octanol/water partition coefficients are generally greater than 5, which are consistent with the very low water solubility determined both experimentally and by computer modeling.

It should be noted that measurement and prediction of physical/chemical properties for chemicals with surfactant properties such as the FND Nitriles Category chemicals are complicated by their behavior in test systems and the environment, including strong adsorption and absorption properties and surface tension activity. The available measured and modeled data for defining the physical/chemical properties of the FND Nitriles Category chemicals are adequate to meet the SIDS/HPV requirements. No additional studies are proposed for the melting point, boiling point, vapor pressure, partition coefficient and water solubility endpoints for the FND Nitriles Category (see Table 4).

Environmental Fate and Ecotoxicity Reliable Data and SAR Estimates

The available reliable data and SAR estimates for environmental fate and effects of the FND Nitriles Category chemicals are presented in Table 3. Robust Summaries for the reliable studies and model determinations are provided in Appendix A. The Test Plan for Environmental Fate and Ecotoxicity Data is outlined in Table 5.

Photodegradation in air was calculated using the Atkinson method and reported in IUCLID summaries for two chemicals (CAS RNs 638-65-3 and 61790-28-1). These data indicated a rapid degradation ($t_{1/2}$ < 1.5 days). Similarly, AOPWIN estimates for eight of the remaining

category chemicals indicated estimated half-lives between approximately 1 and 11 hours. Thus, although the low volatility indicates that the FND Nitriles Category chemicals are unlikely to exist in air, they would be expected to degrade rapidly upon exposure to ambient light.

The HYDROWIN submodel did not provide estimates of stability in water for this class of chemicals because the model cannot calculate this parameter for chemicals that do not meet the criteria of neutral organic compounds with structures that can be hydrolyzed. These types of long-chain hydrocarbon derivatives are generally not hydrolysable.

An estimation of the transport and distribution of the FND Nitriles Category chemicals in environmental media (percent in air, water, soil and sediment) following entry into the environment via water is presented in Table 3. Except for dodecanenitrile, the only member of the category with an estimated water solubility > 1 mg/L, the predictions indicated high distribution to the sediment (≥ 77%) with the remainder mostly distributed to water and virtually no distribution to air and soil. For dodecanenitrile, the prediction was for higher distribution to water (~ 67%) with the remainder primarily to sediment.

Measured values for biodegradation varied from relatively slow (15% in 28 days for CAS RN 2437-25-4) to readily biodegradable (> 70% in 28 days for CAS RNs 61789-53-5, 61790-29-2, and 61790-28-1). The lowest reported value for biodegradation was for the lowest molecular weight (shortest chain length) FND nitrile, dodecanenitrile. This result reflects the complexity in evaluating biodegradation of molecules with surfactant-like properties that adsorb and absorb to microbes, organic material, and other surfaces. In addition, two OECD 301B tests were conducted for CAS RN 61789-53-5. In the first, only 25% (10 mg test chemical/L) and 45% (20 mg test chemical /L) degradation was seen at 28 days. In the second, 71% degradation was attained at 28 days and the criteria were met for ready biodegradation. These results exemplify the complexities in determining the environmental fate and effects of these types of chemicals. Overall, it is reasonable to conclude from the available data that biodegradation of these chemicals occurs and the rate is dependent on the bioavailability and adaptation of the microorganisms.

Measured LC_{50} values for acute toxicity to fish ranged from > 1 to < 100 mg/l, and modeled values all were < 0.1 mg/l. For one of the FND Nitriles Category chemicals (CAS RN 68513-04-2) the ECOSAR model predicted "not toxic at solubility" for fish and did not provide an estimate for aquatic invertebrates or plants. In addition, for CAS RN 26351-32-6, the model predicted "not toxic at solubility" for all three aquatic species. Measured EC_{50} data for acute toxicity to invertebrates for three chemicals (CAS RNs 61789-53-5, 61790-29-2, and 61790-28-1) ranged from 0.005 to 0.26 mg/l and a single measured value for acute toxicity to aquatic plants was 0.497 mg/l (CAS RN 61790-28-1).

Summary – Environmental Fate and Ecotoxicity

Atmospheric photodegradation was predicted to be rapid although fugacity models and the use of FND Nitriles Category chemicals in closed systems suggest minimal potential for distribution of these chemicals to the air. Fugacity models are of limited value for these closed-system intermediates but indicate that all but one (with substantial distribution to water) of the FND Nitriles Category Chemicals would be expected to distribute to sediment in the unlikely event of

environmental exposure. This conclusion is also supported by the limited water solubility of FND Nitriles Category chemicals. Biodegradation data indicate that the FND Nitriles Category chemicals are degradable and accidental release would not pose a long-term environmental contamination concern. From the available data, the FND Nitriles Category chemicals are more toxic to aquatic invertebrates and plants than to fish. This pattern of toxicity is similar to other FND chemicals (amines, cationics, and amides submitted in separate HPV categories) and the relatively high toxicity is likely related to the surfactant-like properties of these chemicals. The FND Nitriles Category chemicals are closed-system intermediates with potential environmental release generally limited to accidents. Therefore, the available data are considered adequate in the HPV screening program to evaluate the environmental fate and ecotoxicity for the entire category (Table 5).

Human Health-Related Reliable Data

The human health-related effects data for SIDS endpoints of the FND Nitriles Category chemicals are limited due to the use of these products as closed-system intermediates. Robust Summaries for the reliable studies are provided in Appendix A. The Test Plan for Human Health-Related Data is outlined in Table 6.

Acute rat oral toxicity LD_{50} data were available for five of the 14 FND Nitriles Category chemicals. The LD_{50} values available were for CAS RNs 2437-25-4, (> 2.0 and ≈ 3.4 g/kg), 112-91-4 (> 5.0 g/kg), 61789-53-5 (>2.0 g/kg), 61790-29-2 (>2.0 g/kg), and 61790-28-1 (>2.0, >5.0, and > 6.0 g/kg). Thus the rat oral LD_{50} values are all greater than 2 g/kg indicating that these chemicals possess slight to negligible acute toxicity by the oral route.

In vitro genetic toxicity studies (*Salmonella* reverse mutation assay) for two of the FND Nitriles Category chemicals (CAS RNs 2437-25-4 and 61790-28-1) were identified. Both tests indicated an absence of mutagenic activity. The data indicate that the FND Nitriles Category chemicals are unlikely to be mutagenic. No chromosomal aberration data are available for the FND Nitriles Category chemicals.

Repeated dose and reproductive toxicity data are not required under the EPA HPV Chemicals Challenge Program for closed-system intermediates. Absence of these studies for the FND Nitriles Category chemicals is not considered to be a data gap.

No developmental toxicity data were available for the FND Nitriles Category chemicals.

Summary – Human Health Related Data

The High Production Volume Chemical Challenge Program design allows for a reduced testing program for closed-system intermediates defined as follows: *"The reduced testing consists of the Screening Information Data Set (SIDS) minus the tests for repeated dose toxicity and reproductive toxicity, but including a developmental toxicity test."* Adequate studies are available to indicate a low level of acute toxicity across the category. As expected, bacterial mutagenicity studies for chemicals of this type and molecular weight were negative. However, no chromosomal aberration studies were available and an evaluation of this endpoint is considered necessary to complete the review of potential mutagenicity under the program. There

were no developmental toxicity data available; therefore, a determination for this endpoint is required for the program. As noted in the discussion above for the category justification, all of the chemicals in the category can be considered very similar. That is, the differences in chain length, degree of saturation of the carbon chains, source of the natural oils, or addition of an amino group in the chain would not be expected to have an impact on the toxicity profile. This conclusion is supported by a number of studies in the FND family of chemicals (amines, cationics, and amides submitted as separate categories) that show no differences in the length or degree of saturation of the alkyl substituents and is also supported by the limited toxicity of these long-chain substituted chemicals. Therefore, the shortest chain substituent, dodecanenitrile, is selected as the category representative for testing because it will provide for the highest degree of bioavailability. The OECD 473 and OECD 421 studies are proposed.

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Meylan, W. and P. H. Howard. 1999b. User's Guide for KOWWIN, Version 1.6. Syracuse Research Corporation, North Syracuse, NY.

Meylan, W. and P. H. Howard. 1999c. User's Guide for WSKOWWIN, Version 1.3. Syracuse Research Corporation, North Syracuse, NY.

Meylan, W. and P. H. Howard. 2000. User's Guide for AOPWIN, Version 1.9. Syracuse Research Corporation, North Syracuse, NY.

Syracuse Research Corporation. 2000. Users Guide for Estimation Programs Interface for Windows, Version 3. Syracuse Research Corporation, North Syracuse, NY.

U. S. EPA. 1999a. Guidance for Testing Closed System Intermediates for the HPV Challenge Program. http://www.epa.gov/chemrtk/sarfinl1.htm.

U. S. EPA. 1999b. Draft Guidance on Developing Robust Summaries. http://www.epa.gov/chemrtk/robsumgd.htm.

U. S. EPA. 1999c. The Use of Structure-activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program. http://www.epa.gov/chemrtk/sarfinl1.htm.

U. S. EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). U.S. Environmental Protection Agency, Washington, DC.

Table 1: Structures of FND Nitriles Category Chemicals

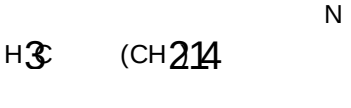
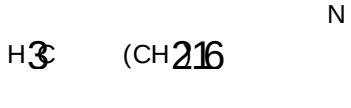
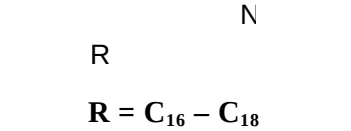
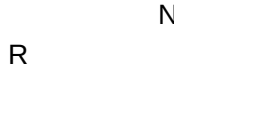
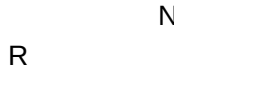
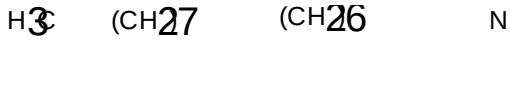
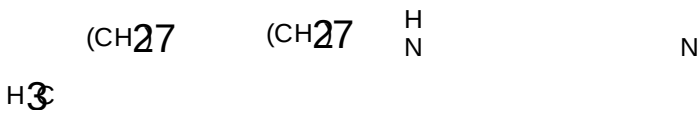
 Dodecanenitrile 2437-25-4	 Hexadecanenitrile 629-79-8
 Octadecanenitrile 638-65-3	 **R = C_{16} – C_{18}** Nitriles, C16-18 68002-65-3
 **R = C_{16} – C_{22}** Nitriles, C16-22 68153-02-6	 **R = C_{14} – C_{18} and C_{16} – C_{18} unsaturated** Nitriles, C14-18 and C16-18-unsatd. 68513-04-2
 **R = C_{16} and C_{18} unsaturated** Nitriles, C16 and C18 unsatd 68002-64-2	 9-Octadecenenitrile 112-91-4
 Propanenitrile, 3-(9-Octadecenylamino)-, (Z)- 26351-32-6	 **R = coco** Nitriles, coco 61789-53-5

Table 1: Structures of FND Nitriles Category Chemicals

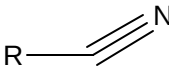
 **R = tallow, hydrogenated** Nitriles, tallow, hydrogenated 61790-29-2	 **R = tallow** Nitriles, tallow 61790-28-1
 **R = tallow alkyl derivs.** Propanenitrile, 3-amino-, N-tallow alkyl derivs. 68784-70-3	 **R = soya** Nitriles, soya 68514-67-0

Table 2: Physical/Chemical Properties Data for FND Nitriles Category Chemicals

CAS RN	Melting Point (°C)	Boiling Point (°C)	Vapor Pressure (mm Hg)	Partition Coefficient (log K_{ow})	Water Solubility (mg/l)
2437-25-4	25	277	0.006	**4.9**	1.9
629-79-8	72	334	0.0003	**> 6**	0.11
638-65-3	**41**	**362**	0.00005	**> 6**	**insoluble**
68002-65-3	81	346	0.0001	7.2	0.009
68153-02-6	99	369	9 E-6	8.2	0.0009
68513-04-2	57	345	0.00009	6.1	0.10
68002-64-2	87	365	0.00001	7.3	0.007
112-91-4	**-1**	**330 – 335 (decomposes)**	0.0004	7.5	**insoluble**
26351-32-6	148	418	2 E-7	7.5	0.02
61789-53-5	**4 < -22**	**220 – 380**	**£ 0.00038**[a]	**5.0**	**practically insoluble**
61790-29-2					
61790-28-1	**1 – 10 5**	**290 – 390**	**0.002**[b]	**5.08**	**not soluble**
68784-70-3					
68514-67-0					

Note: Bold print indicates reliable data for which a Robust Summary is provided in Appendix A.
Regular font indicates data obtained from appropriate models for which Robust Summaries are provided in Appendix A.
Empty block denotes data either are not available or are available and judged inadequate.

[a] Vapor pressure at 50 °C

[b] Vapor pressure at 200 °C

Table 3: Environmental Fate and Ecotoxicity Data for FND Nitriles Category Chemicals

CAS RN	Photodegradation (cm^3/molecule-sec for k_{phot})	Stability in Water	Transport & Distribution	Biodegradation	Acute Toxicity Fish LC_{50} (mg/l)	Acute Toxicity Invertebrates EC_{50} (mg/l)	Acute Toxicity Aquatic Plants EC_{50} (mg/l)
2437-25-4	k_{phot} = 11.6 E-12 $t_{½}$= 11.1 hr	NC	air: 3.0% water: 66.8% soil: < 1% sediment: 30.2%	**15% ThOD in 28 d**	**> 1 < 10**	0.33	0.24
629-79-8	k_{phot} = 17 E-12 $t_{½}$= 7.46 hr	NC	air: < 1% water: 21.9% soil: < 1% sediment: 77.6%		0.031	0.043	0.034
638-65-3	**50% after 0.8 d**	NC	air: < 1% water: 21.9% soil: < 1% sediment: 77.6%		0.034	0.048	0.038
68002-65-3	k_{phot} = 18.6 E-12 $t_{½}$= 6.89 hr	NC	air: < 1% water: 10.9% soil: < 1% sediment: 89%		0.002	0.004	0.003
68153-02-6	k_{phot} = 21.5 E-12 $t_{½}$= 6.0 hr	NC	air: < 1% water: 10.2% soil: < 1% sediment: 89.8%		0.0003	0.0005	0.00045
68513-04-2	k_{phot} = 140 E-12 $t_{½}$= 0.92 hr	NC	air: < 1% water: 20.2% soil: < 1% sediment: 79.8%		not toxic at solubility	not calculable	not calculable
68002-64-2	k_{phot} = 134 E-12 $t_{½}$= 0.96 hr	NC	air: < 1% water: 10.8% soil: < 1% sediment: 89.2%		0.002	0.003	0.003

Note: Bold print indicates reliable data for which a Robust Summary is provided in Appendix A.
Regular font indicates data obtained from appropriate models as described in the text and Appendix A.

Empty block denotes data either are not available or are available and judged inadequate.
NC = Not calculable for FND Nitriles Category chemicals with the HYDROWIN submodel.

Table 3: Environmental Fate and Ecotoxicity Data for FND Nitriles Category Chemicals

CAS RN	Photodegradation (cm^3/molecule-sec for k_{phot})	Stability in Water	Transport & Distribution	Biodegradation	Acute Toxicity Fish LC_{50} (mg/l)	Acute Toxicity Invertebrates EC_{50} (mg/l)	Acute Toxicity Aquatic Plants EC_{50} (mg/l)
112-91-4	k_{phot} = 77 E-12 $t_{½}$= 1.67 hr	NC	air: < 1% water: 10.6% soil: < 1% sediment: 89.4%		0.0013	0.002	0.0018
26351-32-6	k_{phot} = 91 E-12 $t_{½}$= 1.41 hr	NC	air: < 1% water: 5.0% soil: < 1% sediment: 95.0%		not toxic at solubility	not toxic at solubility	not toxic at solubility
61789-53-5				**43% $ThCO_2$ in 28d** **71% $ThCO_2$ in 28d**	**3.53**	**0.033** **0.091**	
61790-29-2				**110% ThOD in 28 d**		**0.216**	
61790-28-1	**50% after 1.4 d (C_{12})** **50% after 0.7 d (C_{20})**			**69% and 78% in 28 and 42 d, respectively** **64% $ThCO_2$ in 28 d** **72% $ThCO_2$ in 28 d**	**> 10 < 100**	**0.005** **0.26**	**0.497**
68784-70-3							
68514-67-0					**33.2**		

Note: Bold print indicates reliable data for which a Robust Summary is provided in Appendix A.
Regular font indicates data obtained from appropriate models as described in the text and Appendix A.

Empty block denotes data either are not available or are available and judged inadequate.
NC = Not calculable for FND Nitriles Category chemicals with the HYDROWIN submodel.

Table 4: Proposed Test Plan for American Chemistry Council FND Nitriles Category Physical/Chemical Properties

CAS RN	Melting Point	Boiling Point	Vapor Pressure	Partition Coefficient (log Kow)	Water Solubility
2437-25-4	M	M	M	**A**	M
629-79-8	M	M	M	**A**	M
638-65-3	**A**	**A**	M	**A**	**A**
68002-65-3	M	M	M	M	M
68153-02-6	M	M	M	M	M
68513-04-2	M	M	M	M	M
68002-64-2	M	M	M	M	M
112-91-4	**A**	**A**	M	M	**A**
26351-32-6	M	M	M	M	M
61789-53-5	**A**	**A**	**A**	**A**	**A**
61790-29-2	C	C	C	C	C
61790-28-1	**A**	**A**	**A**	**A**	**A**
68784-70-3	C	C	C	C	C
68514-67-0	C	C	C	C	C

Note: A = Endpoint fulfilled by adequate reliable data or model data.
M = Endpoint fulfilled by model data.
C = Endpoint fulfilled by category read-across.

Table 5: Proposed Test Plan for American Chemistry Council FND Nitriles Category
Environmental Fate and Ecotoxicity

CAS RN	Photodegradation	Stability in Water	Transport & Distribution	Biodegradation	Acute Tox. to Fish	Acute Tox. to Invertebrates	Toxicity to Aquatic Plants
2437-25-4	M	NC	M	**A**	**A**	M	M
629-79-8	M	NC	M	C	M	M	M
638-65-3	A	NC	M	C	M	M	M
68002-65-3	M	NC	M	C	M	M	M
68153-02-6	M	NC	M	C	M	M	M
68513-04-2	M	NC	M	C	M	M	NC
68002-64-2	M	NC	M	C	M	M	M
112-91-4	M	NC	M	C	M	M	M
26351-32-6	M	NC	M	C	M	M	NC
61789-53-5	C		C	**A**	**A**	**A**	C
61790-29-2	C		C	**A**	C	**A**	C
61790-28-1	**A**		C	**A**	**A**	**A**	**A**
68784-70-3	C		C	C	C	C	C
68514-67-0	C		C	C	**A**	C	C

Note: A = Endpoint fulfilled by adequate reliable data or model data.
M = Endpoint fulfilled by model data.
C = Endpoint fulfilled by category read-across from existing or proposed test data.
NC = cannot be calculated; no measured data available
Empty block denotes data either are not available or are available and judged inadequate.

Table 6: Proposed Test Plan for American Chemistry Council FND Nitriles Category
Human Health-Related Data

CAS RN	Acute Oral Toxicity	Acute Dermal Toxicity	Repeated Dose Toxicity	Genetic Toxicity In vitro	Toxicity to Reproduction	Developmental Toxicity
2437-25-4	**A**	C	NR	**A/OECD 473**	NR	**OECD 421**
629-79-8	C	C	NR	C	NR	C
638-65-3	C	C	NR	C	NR	C
68002-65-3	C	C	NR	C	NR	C
68153-02-6	C	C	NR	C	NR	C
68513-04-2	C	C	NR	C	NR	C
68002-64-2	C	C	NR	C	NR	C
112-91-4	**A**	C	NR	C	NR	C
26351-32-6	C	C	NR	C	NR	C
61789-53-5	**A**	C	NR	C	NR	C
61790-29-2	**A**	C	NR	C	NR	C
61790-28-1	**A**	C	NR	**A**	NR	C
68784-70-3	C	C	NR	C	NR	C
68514-67-0	C	C	NR	C	NR	C

Note: Reliable data for acute toxicity by the oral route of exposure are considered adequate for other routes of exposure.
A = Endpoint fulfilled by adequate reliable data or model data.
OECD = Specified test guideline for proposed study.
C = Endpoint fulfilled by category read-across from existing or proposed test data.
NR = Not required for closed-system intermediates

FND Nitriles HPV Chemicals Challenge

Appendix A

Robust Summaries for Reliable Studies and SAR Model Data

December 29, 2003

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ACC FND HPV Nitriles

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2.1 MELTING POINT

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2.1 MELTING POINT

Test Substance

Identity:	Dodecanenitrile (CAS RN 2437-25-4)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: octanol-water partition coefficient, Log K_{ow} = 4.9.

Results

Melting Point:	25°C
Decomposition:	NA
Sublimation:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:
  Name     :  LAURONITRILE
  CAS Num  :  002437-25-4
  Exp MP (deg C):  4
  Exp BP (deg C):  277
  Exp VP (mm Hg):  2.36E-03  (extrapolated)
  Exp VP (deg C):  25
  Exp VP ref    :  BOUBLIK,T ET AL. (1984)

SMILES : C(#N)CCCCCCCCCC
CHEM   : Dodecanenitrile
MOL FOR: C12 H23 N1
MOL WT : 181.32
----------------- SUMMARY MPBPWIN v1.40 --------------------

Melting Point:   16.83 deg C (Adapted Joback Method)
Melting Point:   48.24 deg C (Gold and Ogle Method)
Mean Melt Pt :   32.54 deg C (Joback; Gold,Ogle Methods)
  Selected MP:   24.68 deg C (Weighted Value)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   -5.10  |   -5.10
 Group | 10  |  -CH2-             |   11.27  |  112.70
 Group |  1  |  -CN  (cyano)      |   59.89  |   59.89
   *   |     |  Equation Constant |          |  122.50
=============+====================+==========+=========
   RESULT    |  MELTING POINT in deg Kelvin  |  289.99
             |  MELTING POINT in deg C       |   16.83
```

- -

Conclusions

The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed: May 21, 2003
Order Number for Sorting:
Remarks:

2.1 MELTING POINT

Test Substance

Identity:	Hexadecanenitrile (CAS RN 629-79-8)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: octanol-water partition coefficient, Log K_{ow} = 6.0.

Results

Melting Point:	72°C
Decomposition:	NA
Sublimation:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:
  Name     :  Hexadecanenitrile
  CAS Num  :  000629-79-8
  Exp MP (deg C):  31
  Exp BP (deg C):  333
  Exp VP (mm Hg):  ---

SMILES : C(#N)CCCCCCCCCCCCCCC
CHEM   : Hexadecanenitrile
MOL FOR: C16 H31 N1
MOL WT : 237.43
------------------- SUMMARY MPBPWIN v1.40 ------------------

Melting Point:   61.91 deg C (Adapted Joback Method)
Melting Point:   81.44 deg C (Gold and Ogle Method)
Mean Melt Pt :   71.68 deg C (Joback; Gold,Ogle Methods)
  Selected MP:   71.68 deg C (Mean Value)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   -5.10  |   -5.10
 Group | 14  |  -CH2-             |   11.27  |  157.78
 Group |  1  |  -CN  (cyano)      |   59.89  |   59.89
   *   |     |  Equation Constant |          |  122.50
=============+====================+==========+=========
   RESULT    |  MELTING POINT in deg Kelvin  |  335.07
             |  MELTING POINT in deg C       |   61.91
-----------------------------------------------------
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability: 2

Remarks: Reliable with restrictions; model data.

References Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed: May 21, 2003

Order Number for Sorting:

Remarks:

2.1 MELTING POINT

Test Substance

Identity:	Octadecanenitrile (CAS RN 638-65-3)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Not stated
GLP:	Not stated
Year:	Not stated
Remarks:	

Results

Melting Point:	41 °C
Decomposition:	Not stated
Sublimation:	Not stated
Remarks:	

Conclusions

Remarks:	The melting point was provided in a reliable resource book. The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions, endpoint was provided in a reliable reference text.

References

Weast, R. C. and M. J. Astle, eds. 1980. CRC Handbook of Chemistry and Physics. CRC Press, Inc., Boca Raton, FL, U. S.

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	3
Remarks:	

2.1 MELTING POINT

Test Substance

Identity:	Nitriles, C16-18 (CAS RN 68002-65-3)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Melting Point:	81°C
Decomposition:	NA
Sublimation:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:
  Name     :  Heptadecanenitrile
  CAS Num  :  005399-02-0
  Exp MP (deg C):  34
  Exp BP (deg C):  349
  Exp VP (mm Hg):  ---

SMILES : C(#N)CCCCCCCCCCCCCCC
CHEM   : Nitriles, C16-18
MOL FOR: C17 H33 N1
MOL WT : 251.46
---------------- SUMMARY MPBPWIN v1.40 ---------------

Melting Point:   73.18 deg C (Adapted Joback Method)
Melting Point:   88.46 deg C (Gold and Ogle Method)
Mean Melt Pt :   80.82 deg C (Joback; Gold,Ogle Methods)
  Selected MP:   80.82 deg C (Mean Value)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   -5.10  |   -5.10
 Group | 15  |  -CH2-             |   11.27  |  169.05
 Group |  1  |  -CN  (cyano)      |   59.89  |   59.89
   *   |     |  Equation Constant |          |  122.50
=============+====================+==========+=========
   RESULT    |  MELTING POINT in deg Kelvin  |  346.34
             |  MELTING POINT in deg C       |   73.18
-----------------------------------------------------
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed: May 22, 2003
Order Number for Sorting:
Remarks:

2.1 MELTING POINT

Test Substance

Identity:	Nitriles, C16-22 (CAS RN 68153-02-6)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Melting Point:	99°C
Decomposition:	NA
Sublimation:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : C(#N)CCCCCCCCCCCCCCCCC
CHEM   : Nitriles, C16-22
MOL FOR: C19 H37 N1
MOL WT : 279.51
---------------------- SUMMARY MPBPWIN v1.40 -------------------

Melting Point:   95.72 deg C (Adapted Joback Method)
Melting Point:  102.01 deg C (Gold and Ogle Method)
Mean Melt Pt :   98.87 deg C (Joback; Gold,Ogle Methods)
  Selected MP:   98.87 deg C (Mean Value)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   -5.10  |   -5.10
 Group | 17  |  -CH2-             |   11.27  |  191.59
 Group |  1  |  -CN  (cyano)      |   59.89  |   59.89
   *   |     |  Equation Constant |          |  122.50
=============+====================+==========+=========
   RESULT    |  MELTING POINT in deg Kelvin  |  368.88
             |  MELTING POINT in deg C       |   95.72
-----------------------------------------------------------
```

Conclusions

The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed: May 23, 2003
Order Number for Sorting:
Remarks:

2.1 MELTING POINT

Test Substance

Identity:	Nitriles, C14-18 and C16-18, unsaturated (CAS RN 68513-04-2)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Melting Point:	57°C
Decomposition:	NA
Sublimation:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : C(#N)CC=CC=CCCCC=CCCCCC
CHEM   : Nitriles, C14-18 and C16-18-unsatd.
MOL FOR: C16 H25 N1
MOL WT : 231.38
------------------ SUMMARY MPBPWIN v1.40 --------------------

Melting Point:   46.67 deg C (Adapted Joback Method)
Melting Point:   87.95 deg C (Gold and Ogle Method)
Mean Melt Pt :   67.31 deg C (Joback; Gold,Ogle Methods)
  Selected MP:   56.99 deg C (Weighted Value)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   -5.10  |   -5.10
 Group |  8  |  -CH2-             |   11.27  |   90.16
 Group |  6  |  =CH-              |    8.73  |   52.38
 Group |  1  |  -CN  (cyano)      |   59.89  |   59.89
   *   |     |  Equation Constant |          |  122.50
=============+====================+==========+=========
   RESULT    |  MELTING POINT in deg Kelvin  |  319.83
             |  MELTING POINT in deg C       |   46.67
-----------------------------------------------------
```

Conclusions

The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed: May 23, 2003
Order Number for Sorting:
Remarks:

2.1 MELTING POINT

Test Substance

Identity:	Nitriles, C16 and C18 unsaturated (CAS RN 68002-64-2)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Melting Point:	87°C
Decomposition:	NA
Sublimation:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : C(#N)CCCCCCCC=CCC=CCCCCC
CHEM   : Nitriles, C16 and C18-unsatd.
MOL FOR: C18 H31 N1
MOL WT : 261.45
---------------------- SUMMARY MPBPWIN v1.40 ---------------

Melting Point:   74.29 deg C (Adapted Joback Method)
Melting Point:   99.41 deg C (Gold and Ogle Method)
Mean Melt Pt :   86.85 deg C (Joback; Gold,Ogle Methods)
  Selected MP:   86.85 deg C (Mean Value)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   -5.10  |   -5.10
 Group | 12  |  -CH2-             |   11.27  |  135.24
 Group |  4  |  =CH-              |    8.73  |   34.92
 Group |  1  |  -CN  (cyano)      |   59.89  |   59.89
   *   |     |  Equation Constant |          |  122.50
=============+====================+==========+=========
   RESULT    |  MELTING POINT in deg Kelvin  |  347.45
             |  MELTING POINT in deg C       |   74.29
-----------------------------------------------------
```

Conclusions

The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed: May 23, 2003
Order Number for Sorting:
Remarks:

2.1 MELTING POINT

Test Substance

Identity:	Oleonitrile (CAS RN 112-91-4; 9-Octadecenenitrile)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Not stated
GLP:	Not stated
Year:	Not stated
Remarks:	

Results

Melting Point:	-1 °C
Decomposition:	Not stated
Sublimation:	Not stated
Remarks:	

Conclusions

Remarks:	The melting point was provided in a reliable resource book. The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	The melting point was provided in a reliable resource book. The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

References

Weast, R. C. and M. J. Astle, eds. 1980. CRC Handbook of Chemistry and Physics. CRC Press, Inc., Boca Raton, FL, U. S.

Other Available Reports

Other

Last Changed:	May 23, 2003
Order Number for Sorting:	1
Remarks:	

2.1 MELTING POINT

Test Substance

Identity:	Propionitrile, 3-(9-Octadecenylamino)- [CAS RN 26351-32-6; Propanenitrile, 3-(9-Octadecenylamino)-, (Z)-]
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Melting Point:	148°C
Decomposition:	NA
Sublimation:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : C(#N)CCNCCCCCCCCC=CCCCCCCCC
CHEM   : Propionitrile, 3-(9-octadecenylamino)-
MOL FOR: C21 H40 N2
MOL WT : 320.57
---------------------- SUMMARY MPBPWIN v1.40 -----------------

Melting Point:  165.84 deg C (Adapted Joback Method)
Melting Point:  130.32 deg C (Gold and Ogle Method)
Mean Melt Pt :  148.08 deg C (Joback; Gold,Ogle Methods)
  Selected MP:  148.08 deg C (Mean Value)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   -5.10  |   -5.10
 Group | 17  |  -CH2-             |   11.27  |  191.59
 Group |  2  |  =CH-              |    8.73  |   17.46
 Group |  1  |  >NH (nonring)     |   52.66  |   52.66
 Group |  1  |  -CN  (cyano)      |   59.89  |   59.89
   *   |     |  Equation Constant |          |  122.50
=============+====================+==========+=========
   RESULT    |  MELTING POINT in deg Kelvin  |  439.00
             |  MELTING POINT in deg C       |  165.84
-------------------------------------------------------
```

Conclusions

The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed: May 26, 2003
Order Number for Sorting:
Remarks:

2.1 MELTING POINT

Test Substance

Identity:	Coco nitrile (CAS RN 61789-53-5; Nitriles, coco)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Not stated
GLP:	Not stated
Year:	Not stated
Remarks:	

Results

Melting Point:	Approximately 4 °C
Decomposition:	Not stated
Sublimation:	Not stated
Remarks:	

Conclusions

Remarks:	The melting point was provided in a reliable resource book. The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions, endpoint provided in a reliable source.

References

Jenkins, W. R. 1992. CESIO 40: Assessment of its ready biodegradability - Modified Sturm Test. Life Science Research Limited, Eye, Suffolk, UK.

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	6
Remarks:	

2.1 Melting Point

Test Substance

Identity:	Nitrile C Dist (CAS RN 61789-53-5; Nitriles, coco)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Directive 84/449/CEE, A.1 and Ligne directrice 102 de l'OCDE
GLP:	1994
Year:	Not stated
Remarks:	

Results

Melting Point:	< -22 °C
Decomposition:	Not stated
Sublimation:	Not stated
Remarks:	

Conclusions

Remarks:	The endpoint was adequately characterized . (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restrictions; guideline study (OECD).

References

Gode, O. and E Bouchet. 1994. Determination de constants physico-chimiques sur Nitriles S et C. Study number 55.94.015. CECA Laboratories.

Other Available Reports

Other

Last Changed:	April 17, 2001
Order Number for Sorting:	20c
Remarks:	

2.1 MELTING POINT

Test Substance

Identity:	Tallow-nitrile (CAS RN 61790-28-1; Nitriles, tallow)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Not stated
GLP:	No
Year:	Not stated
Remarks:	

Results

Melting Point:	Approximately 1 - 10 °C
Decomposition:	Not stated
Sublimation:	Not stated
Remarks:	

Conclusions

Remarks:	The melting point was provided in a reliable resource book. The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restriction; IUCLID summary of study conducted to guideline.

References

Hoechst. 1992. Safety data sheet (00.12.1992), CECA: Internal document (08.04.1994). Cited in IUCLID (update 23-Oct-95).

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	37
Remarks:	

2.1 Melting Point

Test Substance

Identity:	Nitrile S Dist (CAS RN 61790-28-1; Nitriles, tallow)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Directive 84/449/CEE, A.1 and Ligne directrice 102 de l'OCDE
GLP:	1994
Year:	Not stated
Remarks:	

Results

Melting Point:	5 °C
Decomposition:	Not stated
Sublimation:	Not stated
Remarks:	

Conclusions

Remarks:	The endpoint was adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restrictions; guideline study (OECD).

References

Gode, O. and E. Bouchet. 1994. Determination de constants physico-chimiques sur Nitriles S et C. Study number 55.94.015. CECA Laboratories.

Other Available Reports

Other

Last Changed:	April 17, 2001
Order Number for Sorting:	38e
Remarks:	

2.2 BOILING POINT

Test Substance

Identity:	Dodecanenitrile (CAS RN 2437-25-4)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: octanol-water partition coefficient, Log K_{ow} = 4.9.

Results

Boiling Point:	277°C
Pressure:	NA
Pressure Unit:	NA
Decomposition:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:
  Name     :  LAURONITRILE
  CAS Num  :  002437-25-4
  Exp MP (deg C):  4
  Exp BP (deg C):  277
  Exp VP (mm Hg):  2.36E-03  (extrapolated)
  Exp VP (deg C):  25
  Exp VP ref    :  BOUBLIK,T ET AL. (1984)

SMILES : C(#N)CCCCCCCCCC
CHEM   : Dodecanenitrile
MOL FOR: C12 H23 N1
MOL WT : 181.32
----------------- SUMMARY MPBPWIN v1.40 --------------------

Boiling Point:  277.28 deg C (Adapted Stein and Brown Method)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   21.98  |   21.98
 Group | 10  |  -CH2-             |   24.22  |  242.20
 Group |  1  |  -CN  (cyano)      |  119.16  |  119.16
   *   |     |  Equation Constant |          |  198.18
=============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  |  581.52
RESULT- corr |  BOILING POINT in deg Kelvin  |  550.44
             |  BOILING POINT in deg C       |  277.28
-----------------------------------------------------
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed: May 21, 2003
Order Number for Sorting:
Remarks:

2.2 BOILING POINT

Test Substance

Identity:	Hexadecanenitrile (CAS RN 629-79-8)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: octanol-water partition coefficient, Log K_{ow} = 6.0.

Results

Boiling Point:	334°C
Pressure:	NA
Pressure Unit:	NA
Decomposition:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:
  Name     :  Hexadecanenitrile
  CAS Num  :  000629-79-8
  Exp MP (deg C):  31
  Exp BP (deg C):  333
  Exp VP (mm Hg):  ---

SMILES : C(#N)CCCCCCCCCCCCCC
CHEM   : Hexadecanenitrile
MOL FOR: C16 H31 N1
MOL WT : 237.43
------------------ SUMMARY MPBPWIN v1.40 --------------------

Boiling Point:  334.14 deg C (Adapted Stein and Brown Method)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   21.98  |   21.98
 Group | 14  |  -CH2-             |   24.22  |  339.08
 Group |  1  |  -CN  (cyano)      |  119.16  |  119.16
   *   |     |  Equation Constant |          |  198.18
=============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  |  678.40
RESULT- corr |  BOILING POINT in deg Kelvin  |  607.30
             |  BOILING POINT in deg C       |  334.14
-----------------------------------------------------
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability: 2

Remarks: Reliable with restrictions; model data.

References Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed: May 21, 2003

Order Number for Sorting:

Remarks:

2.2 BOILING POINT

Test Substance

Identity:	Octadecanenitrile (CAS RN 638-65-3)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Not stated
GLP:	Not stated
Year:	Not stated
Remarks:	

Results

Boiling Point:	362°C
Pressure:	Not stated
Pressure Unit:	Not stated
Decomposition:	Not stated
Remarks:	

Conclusions

Remarks:	The boiling point was provided in a reliable resource book. The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions, endpoint was provided in a reliable reference text.

References

Weast, R. C. and M. J. Astle, eds. 1980. CRC Handbook of Chemistry and Physics. CRC Press, Inc., Boca Raton, FL, U. S.

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	3
Remarks:	

2.2 BOILING POINT

Test Substance

Identity:	Nitriles, C16-18 (CAS RN 68002-65-3)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Boiling Point:	346°C
Pressure:	NA
Pressure Unit:	NA
Decomposition:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:
  Name     :  Heptadecanenitrile
  CAS Num  :  005399-02-0
  Exp MP (deg C):  34
  Exp BP (deg C):  349
  Exp VP (mm Hg):  ---

SMILES : C(#N)CCCCCCCCCCCCCCC
CHEM   : Nitriles, C16-18
MOL FOR: C17 H33 N1
MOL WT : 251.46
---------------- SUMMARY MPBPWIN v1.40 ---------------

Boiling Point:  346.17 deg C (Adapted Stein and Brown Method)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   21.98  |   21.98
 Group | 15  |  -CH2-             |   24.22  |  363.30
 Group |  1  |  -CN  (cyano)      |  119.16  |  119.16
   *   |     |  Equation Constant |          |  198.18
=============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  |  702.62
RESULT- corr |  BOILING POINT in deg Kelvin  |  619.33
             |  BOILING POINT in deg C       |  346.17
-----------------------------------------------------
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability: 2

Remarks: Reliable with restrictions; model data.

References Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed: May 22, 2003

Order Number for Sorting:

Remarks:

2.2 BOILING POINT

Test Substance

Identity:	Nitriles, C16-22 (CAS RN 68153-02-6)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Boiling Point:	369°C
Pressure:	NA
Pressure Unit:	NA
Decomposition:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : C(#N)CCCCCCCCCCCCCCCCC
CHEM   : Nitriles, C16-22
MOL FOR: C19 H37 N1
MOL WT : 279.51
---------------------- SUMMARY MPBPWIN v1.40 -------------------

Boiling Point:  369.37 deg C (Adapted Stein and Brown Method)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   21.98  |   21.98
 Group | 17  |  -CH2-             |   24.22  |  411.74
 Group |  1  |  -CN  (cyano)      |  119.16  |  119.16
   *   |     |  Equation Constant |          |  198.18
=============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  |  751.06
RESULT- corr |  BOILING POINT in deg Kelvin  |  642.53
             |  BOILING POINT in deg C       |  369.37
-----------------------------------------------------------
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed:	May 23, 2003
Order Number for Sorting:	
Remarks:	

2.2 BOILING POINT

Test Substance

Identity:	Nitriles, C14-18 and C16-18, unsaturated (CAS RN 68513-04-2)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Boiling Point:	345°C
Pressure:	NA
Pressure Unit:	NA
Decomposition:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : C(#N)CC=CC=CCCCC=CCCCCC
CHEM   : Nitriles, C14-18 and C16-18-unsatd.
MOL FOR: C16 H25 N1
MOL WT : 231.38
------------------ SUMMARY MPBPWIN v1.40 --------------------

Boiling Point:  345.28 deg C (Adapted Stein and Brown Method)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   21.98  |   21.98
 Group |  8  |  -CH2-             |   24.22  |  193.76
 Group |  6  |  =CH-              |   27.95  |  167.70
 Group |  1  |  -CN  (cyano)      |  119.16  |  119.16
   *   |     |  Equation Constant |          |  198.18
=============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  |  700.78
RESULT- corr |  BOILING POINT in deg Kelvin  |  618.44
             |  BOILING POINT in deg C       |  345.28
-----------------------------------------------------
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability: 2

Remarks: Reliable with restrictions; model data.

References Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed: May 23, 2003

Order Number for Sorting:

Remarks:

2.2 BOILING POINT

Test Substance

Identity:	Nitriles, C16 and C18 unsaturated (CAS RN 68002-64-2)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Boiling Point:	365°C
Pressure:	NA
Pressure Unit:	NA
Decomposition:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : C(#N)CCCCCCCC=CCC=CCCCCC
CHEM   : Nitriles, C16 and C18-unsatd.
MOL FOR: C18 H31 N1
MOL WT : 261.45
---------------------- SUMMARY MPBPWIN v1.40 ---------------

Boiling Point:  364.92 deg C (Adapted Stein and Brown Method)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   21.98  |   21.98
 Group | 12  |  -CH2-             |   24.22  |  290.64
 Group |  4  |  =CH-              |   27.95  |  111.80
 Group |  1  |  -CN  (cyano)      |  119.16  |  119.16
   *   |     |  Equation Constant |          |  198.18
=============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  |  741.76
RESULT- corr |  BOILING POINT in deg Kelvin  |  638.08
             |  BOILING POINT in deg C       |  364.92
-----------------------------------------------------
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability: 2

Remarks: Reliable with restrictions; model data.

References Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed: May 23, 2003

Order Number for Sorting:

Remarks:

2.2 BOILING POINT

Test Substance

Identity:	Oleonitrile (CAS RN 112-91-4; 9-Octadecenenitrile)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Not stated
GLP:	Not stated
Year:	Not stated
Remarks:	

Results

Boiling Point:	Approximately 330 – 335 (decomposes)
Pressure:	Not stated
Pressure Unit:	Not stated
Decomposition:	None
Remarks:	

Conclusions

Remarks:	The endpoint was adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restriction; IUCLID summary of study conducted to guideline.

References

Weast, R. C., ed. 1979. Physical Constants of Organic Compounds. p. C – 404. CRC Handbook of Chemistry and Physics, 60th ed. CRC Press Inc., Boca Raton, FL, U. S.

Other Available Reports

Other

Last Changed:	May 23, 2003
Order Number for Sorting:	1
Remarks:	

2.2 BOILING POINT

Test Substance

Identity:	Propionitrile, 3-(9-Octadecenylamino)- [CAS RN 26351-32-6; Propanenitrile, 3-(9-Octadecenylamino)-, (Z)-]
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Boiling Point:	418°C
Pressure:	NA
Pressure Unit:	NA
Decomposition:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : C(#N)CCNCCCCCCCCC=CCCCCCCCC
CHEM   : Propionitrile, 3-(9-octadecenylamino)-
MOL FOR: C21 H40 N2
MOL WT : 320.57
---------------------- SUMMARY MPBPWIN v1.40 -----------------

Boiling Point:  417.85 deg C (Adapted Stein and Brown Method)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   21.98  |   21.98
 Group | 17  |  -CH2-             |   24.22  |  411.74
 Group |  2  |  =CH-              |   27.95  |   55.90
 Group |  1  |  >NH (nonring)     |   45.28  |   45.28
 Group |  1  |  -CN  (cyano)      |  119.16  |  119.16
   *   |     |  Equation Constant |          |  198.18
=============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  |  852.24
RESULT- corr |  BOILING POINT in deg Kelvin  |  691.01
             |  BOILING POINT in deg C       |  417.85
-----------------------------------------------------
```

Conclusions

The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed: May 26, 2003
Order Number for Sorting:
Remarks:

2.2 BOILING POINT

Test Substance

Identity:	Coco-nitrile (CAS RN 61789-53-5; Nitriles, coco)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Not stated
GLP:	Not stated
Year:	1987
Remarks:	

Results

Boiling Point:	Approximately 220 – 380°C
Pressure:	1013 hPa
Pressure Unit:	Not stated
Decomposition:	None
Remarks:	

Conclusions

Remarks:	The melting point was provided in a reliable resource book. The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restriction; IUCLID summary of study conducted to guideline.

References

Ralston, A. W. 1941. Ind. and Eng. Chem. 33(5):682 – 683. Cited in IUCLID (update October 23, 1985).

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	20
Remarks:	

2.2 BOILING POINT

Test Substance

Identity:	Tallow-nitrile (CAS RN 61790-28-1; Nitriles, tallow)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Not stated
GLP:	Not stated
Year:	Not stated
Remarks:	

Results

Boiling Point:	Approximately 290 – 390°C
Pressure:	1013 hPa
Pressure Unit:	Not stated
Decomposition:	None
Remarks:	

Conclusions

Remarks:	The boiling point was provided in a reliable resource book. The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restriction; IUCLID summary of study conducted to guideline.

References

Ralston, A. W. 1941. Ind. and Eng. Chem. 33(5):682 – 683. Cited in IUCLID (update October 23, 1985).

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	37
Remarks:	

2.4 VAPOR PRESSURE

Test Substance

Identity:	Dodecanenitrile (CAS RN 2437-25-4)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: octanol-water partition coefficient, Log K_{ow} = 4.9.

Results

Vapor Pressure:	0.006 mm Hg
Temperature:	25°C
Decomposition:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:
  Name     :  LAURONITRILE
  CAS Num  :  002437-25-4
  Exp MP (deg C):  4
  Exp BP (deg C):  277
  Exp VP (mm Hg):  2.36E-03  (extrapolated)
  Exp VP (deg C):  25
  Exp VP ref    :  BOUBLIK,T ET AL. (1984)

SMILES : C(#N)CCCCCCCCCC
CHEM   : Dodecanenitrile
MOL FOR: C12 H23 N1
MOL WT : 181.32
---------------- SUMMARY MPBPWIN v1.40 --------------------

Vapor Pressure Estimations (25 deg C):
  (Using BP: 277.00 deg C (exp database))
  (MP not used for liquids)
    VP:  0.006 mm Hg (Antoine Method)
    VP:  0.00656 mm Hg (Modified Grain Method)
    VP:  0.012 mm Hg (Mackay Method)
  Selected VP:  0.00628 mm Hg (Mean of Antoine & Grain methods)
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

2.4 VAPOR PRESSURE

Test Substance

Identity:	Hexadecanenitrile (CAS RN 629-79-8)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: octanol-water partition coefficient, Log K_{ow} = 6.0.

Results

Vapor Pressure:	0.000294 mm Hg
Temperature:	25°C
Decomposition:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:
  Name     :  Hexadecanenitrile
  CAS Num  :  000629-79-8
  Exp MP (deg C):  31
  Exp BP (deg C):  333
  Exp VP (mm Hg):  ---

SMILES : C(#N)CCCCCCCCCCCCCCC
CHEM   : Hexadecanenitrile
MOL FOR: C16 H31 N1
MOL WT : 237.43
------------------ SUMMARY MPBPWIN v1.40 --------------------

Vapor Pressure Estimations (25 deg C):
  (Using BP: 333.00 deg C (exp database))
  (Using MP: 31.00 deg C (exp database))
    VP:  0.000168 mm Hg (Antoine Method)
    VP:  0.000294 mm Hg (Modified Grain Method)
    VP:  0.000567 mm Hg (Mackay Method)
  Selected VP:  0.000294 mm Hg (Modified Grain Method)
```

Conclusions	The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability:	2

Remarks: Reliable with restrictions; model data.

References Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed: May 21, 2003
Order Number for Sorting:
Remarks:

2.4 VAPOR PRESSURE

Test Substance

Identity:	Octadecanenitrile (CAS RN 638-65-3)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: melting point = 41°C; boiling point = 362°C; octanol-water partition coefficient, Log K_{ow} = 6.0.

Results

Vapor Pressure:	4.9 E-005 mm Hg
Temperature:	25°C
Decomposition:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:
  Name     :  Octadecanenitrile
  CAS Num  :  000638-65-3
  Exp MP (deg C):  41
  Exp BP (deg C):  362
  Exp VP (mm Hg):  ---

SMILES : C(#N)CCCCCCCCCCCCCCCCC
CHEM   : Octadecanenitrile
MOL FOR: C18 H35 N1
MOL WT : 265.49
----------------- SUMMARY MPBPWIN v1.40 -------------



Vapor Pressure Estimations (25 deg C):
  (Using BP: 362.00 deg C (user entered))
  (Using MP: 41.00 deg C (user entered))
    VP:  1.94E-005 mm Hg (Antoine Method)
    VP:  4.9E-005 mm Hg (Modified Grain Method)
    VP:  9.52E-005 mm Hg (Mackay Method)
  Selected VP:  4.9E-005 mm Hg (Modified Grain Method)
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed:	May 22, 2003
Order Number for Sorting:	
Remarks:	

2.4 VAPOR PRESSURE

Test Substance

Identity:	Nitriles, C16-18 (CAS RN 68002-65-3)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Vapor Pressure:	0.0001 mm Hg
Temperature:	25°C
Decomposition:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:
  Name     :  Heptadecanenitrile
  CAS Num  :  005399-02-0
  Exp MP (deg C):  34
  Exp BP (deg C):  349
  Exp VP (mm Hg):  ---

SMILES : C(#N)CCCCCCCCCCCCCCC
CHEM   : Nitriles, C16-18
MOL FOR: C17 H33 N1
MOL WT : 251.46
---------------- SUMMARY MPBPWIN v1.40 ---------------


Vapor Pressure Estimations (25 deg C):
  (Using BP: 349.00 deg C (exp database))
  (Using MP: 34.00 deg C (exp database))
    VP:  5.47E-005 mm Hg (Antoine Method)
    VP:  0.000116 mm Hg (Modified Grain Method)
    VP:  0.000225 mm Hg (Mackay Method)
  Selected VP:  0.000116 mm Hg (Modified Grain Method)
```

Conclusions	The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability:	2

Remarks:	Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed:	May 22, 2003
Order Number for Sorting:	
Remarks:	

2.4 VAPOR PRESSURE

Test Substance

Identity:	Nitriles, C16-22 (CAS RN 68153-02-6)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Vapor Pressure:	9 E-006 mm Hg
Temperature:	25°C
Decomposition:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : C(#N)CCCCCCCCCCCCCCCCC
CHEM   : Nitriles, C16-22
MOL FOR: C19 H37 N1
MOL WT : 279.51
---------------------- SUMMARY MPBPWIN v1.40 -------------------

Vapor Pressure Estimations (25 deg C):
  (Using BP: 369.37 deg C (estimated))
  (Using MP: 98.87 deg C (estimated))
    VP:  3.11E-006 mm Hg (Antoine Method)
    VP:  8.72E-006 mm Hg (Modified Grain Method)
    VP:  1.71E-005 mm Hg (Mackay Method)
  Selected VP:  8.72E-006 mm Hg (Modified Grain Method)
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed: May 23, 2003
Order Number for Sorting:
Remarks:

2.4 VAPOR PRESSURE

Test Substance

Identity:	Nitriles, C14-18 and C16-18, unsaturated (CAS RN 68513-04-2)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Vapor Pressure:	8.63 E-005 mm Hg
Temperature:	25°C
Decomposition:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : C(#N)CC=CC=CCCCC=CCCCCC
CHEM   : Nitriles, C14-18 and C16-18-unsatd.
MOL FOR: C16 H25 N1
MOL WT : 231.38
------------------ SUMMARY MPBPWIN v1.40 --------------------

Vapor Pressure Estimations (25 deg C):
  (Using BP: 345.28 deg C (estimated))
  (Using MP: 56.99 deg C (estimated))
    VP:  4.27E-005 mm Hg (Antoine Method)
    VP:  8.63E-005 mm Hg (Modified Grain Method)
    VP:  0.000163 mm Hg (Mackay Method)
  Selected VP:  8.63E-005 mm Hg (Modified Grain Method)
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed: May 23, 2003
Order Number for Sorting:
Remarks:

2.4 VAPOR PRESSURE

Test Substance

Identity:	Nitriles, C16 and C18 unsaturated (CAS RN 68002-64-2)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Vapor Pressure:	1.48 E-005 mm Hg
Temperature:	25°C
Decomposition:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : C(#N)CCCCCCCC=CCC=CCCCCC
CHEM   : Nitriles, C16 and C18-unsatd.
MOL FOR: C18 H31 N1
MOL WT : 261.45
---------------------- SUMMARY MPBPWIN v1.40 ---------------

Vapor Pressure Estimations (25 deg C):
  (Using BP: 364.92 deg C (estimated))
  (Using MP: 86.85 deg C (estimated))
    VP:  5.65E-006 mm Hg (Antoine Method)
    VP:  1.48E-005 mm Hg (Modified Grain Method)
    VP:  2.86E-005 mm Hg (Mackay Method)
  Selected VP:  1.48E-005 mm Hg (Modified Grain Method)
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed: May 23, 2003
Order Number for Sorting:
Remarks:

2.4 VAPOR PRESSURE

Test Substance

Identity:	9-Octadecenenitrile, (Z)- (CAS RN 112-91-4)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: melting point = -1°C and boiling point = 330°C.

Results

Vapor Pressure:	0.0004 mm Hg
Temperature:	25°C
Decomposition:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:
  Name     :  9-Octadecenenitrile, (Z)-
  CAS Num  :  000112-91-4
  Exp MP (deg C):  -1
  Exp BP (deg C):  ---
  Exp VP (mm Hg):  ---

SMILES : C(#N)CCCCCCCC=CCCCCCCCC
CHEM   : 9-Octadecenenitrile, (Z)-
MOL FOR: C18 H33 N1
MOL WT : 263.47
---------------- SUMMARY MPBPWIN v1.40 --------------

Vapor Pressure Estimations (25 deg C):
  (Using BP: 330.00 deg C (user entered))
  (MP not used for liquids)
    VP:  0.000231 mm Hg (Antoine Method)
    VP:  0.000391 mm Hg (Modified Grain Method)
    VP:  0.000763 mm Hg (Mackay Method)
  Selected VP:  0.000391 mm Hg (Modified Grain Method)
```

Conclusions

The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability:	2

Remarks:	Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed:	May 23, 2003
Order Number for Sorting:	
Remarks:	

2.4 VAPOR PRESSURE

Test Substance

Identity:	Propionitrile, 3-(9-Octadecenylamino)- [CAS RN 26351-32-6; Propanenitrile, 3-(9-Octadecenylamino)-, (Z)-]
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) MPBPVP Submodel v 1.40
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Vapor Pressure:	1.7 E-007 mm Hg
Temperature:	25°C
Decomposition:	NA
Remarks:	Following are the results from the model:

```
MPBPWIN (v1.40) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : C(#N)CCNCCCCCCCCC=CCCCCCCCC
CHEM   : Propionitrile, 3-(9-octadecenylamino)-
MOL FOR: C21 H40 N2
MOL WT : 320.57
---------------------- SUMMARY MPBPWIN v1.40 -----------------

Vapor Pressure Estimations (25 deg C):
  (Using BP: 417.85 deg C (estimated))
  (Using MP: 148.08 deg C (estimated))
    VP:  2.54E-008 mm Hg (Antoine Method)
    VP:  1.71E-007 mm Hg (Modified Grain Method)
    VP:  3.83E-007 mm Hg (Mackay Method)
  Selected VP:  1.71E-007 mm Hg (Modified Grain Method)
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for MPBPVP, version 1.4; Syracuse Research Corporation, North Syracuse, NY.

Other Available Reports

Other

Last Changed: May 26, 2003
Order Number for Sorting:
Remarks:

2.4 VAPOR PRESSURE

Test Substance

Identity:	Coco-nitrile (CAS RN 61789-53-5; Nitriles, coco)
Purity:	Not stated
Remarks:	Not stated

Method

Method/Guideline followed:	Calculated
GLP:	Not stated
Year:	Not stated
Remarks:	

Results

Vapor Pressure:	5 hPa (0.00038 mm Hg)
Temperature:	50 °C
Decomposition:	Not stated
Remarks:	

Conclusions

Remarks:	The vapor pressure has been adequately characterized by a reputable source (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restriction; IUCLID summary of study conducted to guideline.

References

Ralston, A. W. 1941. Ind. and Eng. Chem. 33(5):682 – 683. Cited in IUCLID (update October 23, 1985).

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	20
Remarks:	

2.4 VAPOR PRESSURE

Test Substance

Identity:	Tallow-nitrile (CAS RN 61790-28-1; Nitriles, tallow)
Purity:	Not stated
Remarks:	Not stated

Method

Method/Guideline followed:	Measured
GLP:	Not stated
Year:	Not stated
Remarks:	

Results

Vapor Pressure:	Approximately 27 hPa (0.002 mm Hg)
Temperature:	200° C
Decomposition:	Not stated
Remarks:	

Conclusions

Remarks:	The vapor pressure has been adequately characterized by a reputable source (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restriction; IUCLID summary of study conducted to guideline.

References

Ralston, A. W. 1941. Ind. and Eng. Chem. 33(5):682 – 683. Cited in IUCLID (update October 23, 1985).

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	37
Remarks:	

2.5 PARTITION COEFFICIENT

Test Substance

Identity:	Dodecanenitrile (CAS RN 2437-25-4)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Calculated
GLP:	No
Year:	1986
Remarks:	Medchem Software CLOGP3, release 3.42

Results

Log P_{ow}:	4.9
Temperature:	25°C
Remarks:	

Conclusions

Remarks:	The partition coefficient of the test substance has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restriction; IUCLID summary of study conducted to guideline.

References

Hoechst. 1992. Berechnung der Abt. UCV (08.07.1992). Cited in IUCLID (update 23-Oct-95).

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	5
Remarks:	

2.5 PARTITION COEFFICIENT

Test Substance

Identity:	Hexadecanenitrile (CAS RN 629-79-8)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Calculated
GLP:	No
Year:	1986
Remarks:	Medchem Software CLOGP3, release 3.42

Results

Log P_{ow}:	> 6
Temperature:	25 °C
Remarks:	

Conclusions

Remarks:	The partition coefficient of the test substance has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restriction; IUCLID summary of study conducted to guideline.

References

Hoechst. 1992. Berechnung der Abt. UCV (08.07.1992). Cited in IUCLID (update 23-Oct-95).

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	39
Remarks:	

2.5 PARTITION COEFFICIENT

Test Substance

Identity:	Octadecanenitrile (CAS RN 638-65-3)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Calculated
GLP:	No
Year:	1986
Remarks:	Medchem Software CLOGP3, release 3.42

Results

Log P_{ow}:	> 6
Temperature:	25 °C
Remarks:	

Conclusions

Remarks:	The partition coefficient of the test substance has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restriction; IUCLID summary of study conducted to guideline.

References

Hoechst. 1992. Berechnung der Abt. UCV (08.07.1992). Cited in IUCLID (update 23-Oct-95).

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	4a
Remarks:	

2.5 PARTITION COEFFICIENT

Test Substance

Identity:	Nitriles, C16-18 (CAS RN 68002-65-3)
Purity:	NA

Method

Method:	EPIWIN (v 3.10) KOWWIN Submodel (v 1.66)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Log K_{ow}:	7.2
Temperature °C:	NA
Remarks:	Following are the results from the model:

```
KOWWIN Program (v1.66) Results:
===============================

                 Log Kow(version 1.66 estimate): 7.22

SMILES : C(#N)CCCCCCCCCCCCCCC
CHEM   : Nitriles, C16-18
MOL FOR: C17 H33 N1
MOL WT : 251.46
-------+-----+---------------------------------------+---------+--------
 TYPE  | NUM |        LOGKOW FRAGMENT DESCRIPTION    |  COEFF  |  VALUE
-------+-----+---------------------------------------+---------+--------
 Frag  |  1  |  -CH3    [aliphatic carbon]           | 0.5473  |  0.5473
 Frag  | 15  |  -CH2-   [aliphatic carbon]           | 0.4911  |  7.3665
 Frag  |  1  |  -C#N    [cyano, aliphatic attach]    |-0.9218  | -0.9218
 Const |     |  Equation Constant                    |         |  0.2290
-------+-----+---------------------------------------+---------+--------
                                                    Log Kow   =   7.2210
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for KOWWIN, version 1.6; Syracuse Research Corporation, North Syracuse, NY

Other

Last changed: May 22, 2003
Order number for sorting:
Remarks:

2.5 PARTITION COEFFICIENT

Test Substance

Identity:	Nitriles, C16-22 (CAS RN 68153-02-6)
Purity:	NA

Method

Method:	EPIWIN (v 3.10) KOWWIN Submodel (v 1.66)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Log K_{ow}:	8.2
Temperature °C:	NA
Remarks:	Following are the results from the model:

```
KOWWIN Program (v1.66) Results:
===============================

                 Log Kow(version 1.66 estimate): 8.20

SMILES : C(#N)CCCCCCCCCCCCCCCCC
CHEM   : Nitriles, C16-22
MOL FOR: C19 H37 N1
MOL WT : 279.51
-------+-----+---------------------------------------+---------+--------
 TYPE  | NUM |        LOGKOW FRAGMENT DESCRIPTION    |  COEFF  |  VALUE
-------+-----+---------------------------------------+---------+--------
 Frag  |  1  |  -CH3    [aliphatic carbon]           | 0.5473  |  0.5473
 Frag  | 17  |  -CH2-   [aliphatic carbon]           | 0.4911  |  8.3487
 Frag  |  1  |  -C#N    [cyano, aliphatic attach]    |-0.9218  | -0.9218
 Const |     |  Equation Constant                    |         |  0.2290
-------+-----+---------------------------------------+---------+--------
                                                    Log Kow   =   8.2032
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for KOWWIN, version 1.6; Syracuse Research Corporation, North Syracuse, NY

Other

Last changed: May 23, 2003
Order number for sorting:
Remarks:

2.5 PARTITION COEFFICIENT

Test Substance

Identity:	Nitriles, C14-18 and C16-18, unsaturated (CAS RN 68513-04-2)
Purity:	NA

Method

Method:	EPIWIN (v 3.10) KOWWIN Submodel (v 1.66)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Log K_{ow}:	6.1
Temperature °C:	NA
Remarks:	Following are the results from the model:

```
KOWWIN Program (v1.66) Results:
===============================

                  Log Kow(version 1.66 estimate): 6.08

SMILES : C(#N)CC=CC=CCCCC=CCCCCC
CHEM   : Nitriles, C14-18 and C16-18-unsatd.
MOL FOR: C16 H25 N1
MOL WT : 231.38
-------+-----+---------------------------------------+---------+--------
 TYPE  | NUM |        LOGKOW FRAGMENT DESCRIPTION    |  COEFF  |  VALUE
-------+-----+---------------------------------------+---------+--------
 Frag  |  1  |  -CH3    [aliphatic carbon]           | 0.5473  |  0.5473
 Frag  |  8  |  -CH2-   [aliphatic carbon]           | 0.4911  |  3.9288
 Frag  |  6  |  =CH- or =C<  [olefinc carbon]        | 0.3836  |  2.3016
 Frag  |  1  |  -C#N    [cyano, aliphatic attach]    |-0.9218  | -0.9218
 Const |     |  Equation Constant                    |         |  0.2290
-------+-----+---------------------------------------+---------+--------
                                                    Log Kow   =   6.0849
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for KOWWIN, version 1.6; Syracuse Research Corporation, North Syracuse, NY

Other

Last changed: May 23, 2003
Order number for sorting:
Remarks:

2.5 PARTITION COEFFICIENT

Test Substance

Identity:	Nitriles, C16 and C18 unsaturated (CAS RN 68002-64-2)
Purity:	NA

Method

Method:	EPIWIN (v 3.10) KOWWIN Submodel (v 1.66)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Log K_{ow}:	7.3
Temperature °C:	NA
Remarks:	Following are the results from the model:

```
KOWWIN Program (v1.66) Results:
===============================

                  Log Kow(version 1.66 estimate): 7.28

SMILES : C(#N)CCCCCCCC=CCC=CCCCCC
CHEM   : Nitriles, C16 and C18-unsatd.
MOL FOR: C18 H31 N1
MOL WT : 261.45
-------+-----+---------------------------------------+---------+--------
 TYPE  | NUM |        LOGKOW FRAGMENT DESCRIPTION    |  COEFF  |  VALUE
-------+-----+---------------------------------------+---------+---
-----
 Frag  |  1  |  -CH3    [aliphatic carbon]           | 0.5473  |  0.5473
 Frag  | 12  |  -CH2-   [aliphatic carbon]           | 0.4911  |  5.8932
 Frag  |  4  |  =CH- or =C<  [olefinc carbon]        | 0.3836  |  1.5344
 Frag  |  1  |  -C#N    [cyano, aliphatic attach]    |-0.9218  | -0.9218
 Const |     |  Equation Constant                    |         |  0.2290
-------+-----+---------------------------------------+---------+--------
                                                     Log Kow   =   7.2821
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for KOWWIN, version 1.6; Syracuse Research Corporation, North Syracuse, NY

Other

Last changed: May 23, 2003
Order number for sorting:
Remarks:

2.5 PARTITION COEFFICIENT

Test Substance

Identity:	9-Octadecenenitrile, (Z)- (CAS RN 112-91-4)
Purity:	NA

Method

Method:	EPIWIN (v 3.10) KOWWIN Submodel (v 1.66)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: melting point = -1°C and boiling point = 330°C.

Results

Log K_{ow}:	7.5
Temperature °C:	NA
Remarks:	Following are the results from the model:

```
KOWWIN Program (v1.66) Results:
===============================

                  Log Kow(version 1.66 estimate): 7.50

SMILES : C(#N)CCCCCCCC=CCCCCCCCC
CHEM   : 9-Octadecenenitrile, (Z)-
MOL FOR: C18 H33 N1
MOL WT : 263.47
-------+-----+---------------------------------------+---------+--------
 TYPE  | NUM |        LOGKOW FRAGMENT DESCRIPTION    |  COEFF  |  VALUE
-------+-----+---------------------------------------+---------+--------
 Frag  |  1  |  -CH3    [aliphatic carbon]           | 0.5473  |  0.5473
 Frag  | 14  |  -CH2-   [aliphatic carbon]           | 0.4911  |  6.8754
 Frag  |  2  |  =CH- or =C<  [olefinc carbon]        | 0.3836  |  0.7672
 Frag  |  1  |  -C#N    [cyano, aliphatic attach]    |-0.9218  | -0.9218
 Const |     |  Equation Constant                    |         |  0.2290
-------+-----+---------------------------------------+---------+--------
                                                     Log Kow   =   7.4971
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for KOWWIN, version 1.6; Syracuse Research Corporation, North Syracuse, NY

Other

Last changed: May 23, 2003
Order number for sorting:
Remarks:

2.5 PARTITION COEFFICIENT

Test Substance

Identity:	Propionitrile, 3-(9-Octadecenylamino)- [CAS RN 26351-32-6; Propanenitrile, 3-(9-Octadecenylamino)-, (Z)-]
Purity:	NA

Method

Method:	EPIWIN (v 3.10) KOWWIN Submodel (v 1.66)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Log K_{ow}:	7.5
Temperature °C:	NA
Remarks:	Following are the results from the model:

```
KOWWIN Program (v1.66) Results:
===============================

                Log Kow(version 1.66 estimate): 7.47

SMILES : C(#N)CCNCCCCCCCCC=CCCCCCCCC
CHEM   : Propionitrile, 3-(9-octadecenylamino)-
MOL FOR: C21 H40 N2
MOL WT : 320.57
-------+-----+-------------------------------------+---------+--------
 TYPE  | NUM |        LOGKOW FRAGMENT DESCRIPTION  |  COEFF  |  VALUE
-------+-----+-------------------------------------+---------+--------
 Frag  |  1  |  -CH3    [aliphatic carbon]         | 0.5473  |  0.5473
 Frag  | 17  |  -CH2-   [aliphatic carbon]         | 0.4911  |  8.3487
 Frag  |  2  |  =CH- or =C<  [olefinc carbon]      | 0.3836  |  0.7672
 Frag  |  1  |  -NH-    [aliphatic attach]         |-1.4962  | -1.4962
 Frag  |  1  |  -C#N    [cyano, aliphatic attach]  |-0.9218  | -0.9218
 Const |     |  Equation Constant                  |         |  0.2290
-------+-----+-------------------------------------+---------+--------
                                                  Log Kow   =   7.4742
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for KOWWIN, version 1.6; Syracuse Research Corporation, North Syracuse, NY

Other

Last changed: May 26, 2003
Order number for sorting:
Remarks:

2.5 PARTITION COEFFICIENT

Test Substance

Identity:	CESIO 44 (CAS RN 61789-53-5; Nitriles, coco)
Purity:	Purity provided as percent distribution of carbon chain lengths from C8 to C18.
Remarks:	

Method

Method/Guideline followed:	Test conducted in accordance with OECD Guidelines for Testing of Chemicals, and EEC Directive 84/449/EEC.
GLP:	Yes
Year:	1992
Remarks:	Partition coefficients were determined by the estimation method of Leo and Hansch (Citation: Lyman, Reehl, and Rosenblatt. 1982. Handbook of Chemical Property Estimation Methods. McGraw-Hill Co.) and by the n-octanol/water shakeflask method (OECD and EEC). The experimental determination of the partition coefficient of the test substance was conducted at 21 °C by shaking measured volumes of distilled water saturated with n-octanol with measured volumes of a solution of the test substance in n-octanol. The two phases were shaken for approximately two minutes then transferred to centrifuge tubes. The solutions were centrifuged at 2500 rpm for five minutes at 20 °C and equilibrated at 21 °C overnight. The phases were separated and the concentrations of the test substance were determined analytically by gas chromatography in both fractions. Seven significant peaks were present in the chromatograms with retention times ranging from 1.7 to 23.6 minutes. The partition coefficient was calculated on the two largest peaks present (peaks 3 and 4), retention times 11.5 and 16.1 minutes, which represented approximately 70% of the test material. The detector calibration was linear for those two peaks in the range 0 to 500 mg/l. Six determinations were made and the mean K_{ow} and log K_{ow} were calculated.

Results

Log P_{ow}:	Based on Peak 3 (C_{12}-alkyl) = 5.00 ± 0.06 Based on Peak 4 (C_{14}-alkyl) = 5.12 ± 0.12
Temperature:	Approximately 21 °C
Remarks:	The estimation method for Log K_{ow} for straight chain alkyl nitriles of C_{12} was determined to be 5.68.

Conclusions

Remarks:	The partition coefficient of the test substance has been adequately characterized by empirical determination. The empirical determination also shows good agreement with an acceptable estimation method (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study (OECD).

References

Cowlyn, T. C. 1992. CESIO 44: Octanol water partition coefficient. Confidential report number 92/CFY004/0098. Life Science Research Limited, Eye, Suffolk, UK.

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	11
Remarks:	

2.5 PARTITION COEFFICIENT

Test Substance

Identity:	CESIO 45 (CAS RN 61790-28-1; Nitriles, tallow)
Purity:	Purity provided as percent distribution of carbon chain lengths from C8 to C18.
Remarks:	

Method

Method/Guideline followed:	Test conducted in accordance with OECD Guidelines for Testing of Chemicals, Method 107, and EEC Directive 84/449/EEC, Method A3
GLP:	Yes
Year:	1992
Remarks:	Partition coefficients were determined by the estimation method of Leo and Hansch (Citation: Lyman, Reehl, and Rosenblatt. 1982. Handbook of Chemical Property Estimation Methods. McGraw-Hill Co.) and by the n-octanol/water shakeflask method (OECD and EEC). The experimental determination of the partition coefficient of the test substance was conducted at 21 °C by shaking measured volumes of distilled water saturated with n-octanol with measured volumes of a solution of the test substance in n-octanol. The two phases were shaken for approximately two minutes then transferred to centrifuge tubes. The solutions were centrifuged at 2500 rpm for five minutes at 20 °C and equilibrated at 21 °C for two days. The phases were separated and the concentrations of the test substance were determined analytically by gas chromatography in both fractions. Three significant peaks were present in the chromatograms with retention times ranging from 4.2 to 10.3 minutes. The partition coefficient was quantitated from the third peak (retention time 10.3 minutes), which accounted for approximately 60% of the components in the test substance. The limit of detection was 0.3 mg/l for peak 3. Six determinations were made and the mean K_{ow} and log K_{ow} were calculated.

Results

Log P_{ow}:	Mean Log K_{ow} = 5.08 ± 0.06
Temperature:	Approximately 21 °C
Remarks:	The estimation method for Log K_{ow} yielded a value of 6.76 (value for C14 chain length).

Conclusions

Remarks:	The partition coefficient of the test substance has been adequately characterized by empirical determination. The empirical determination also shows good agreement with an acceptable estimation method (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction, guideline study (OECD).

References

Cowlyn, T. C. 1992. CESIO 45: Octanol water partition coefficient. Final report number 92/CFY006/0139. Life Science Research Limited, Eye, Suffolk, UK.

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	24
Remarks:	

2.6 WATER SOLUBILITY

Test Substance

Identity:	Dodecanenitrile (CAS RN 2437-25-4)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 310) WSKOWWIN Submodel (V 1.40)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: octanol-water partition coefficient, Log K_{ow} = 4.9.

Results

Value:	1.93 mg/L
Solubility:	Soluble in water
pH value and concentration:	NA
pKa value at 25°C:	NA
Remarks:	Following are the results from the model:

```
Water Sol from Kow (WSKOW v1.40) Results:
=========================================

          Water Sol: 1.927 mg/L

SMILES : C(#N)CCCCCCCCCC
CHEM   : Dodecanenitrile
MOL FOR: C12 H23 N1
MOL WT : 181.32
---------------------- WSKOW v1.40 Results ----------------
Log Kow  (estimated)  :  4.77
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  4.90 (user entered)

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
       (used when Melting Point NOT available)

      Correction(s):         Value
      -------------------   -----
       Nitrile              -0.265

   Log Water Solubility  (in moles/L) :  -4.974
   Water Solubility at 25 deg C (mg/L):  1.927
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for WSKOW, version 1.3; Syracuse Research Corporation, North Syracuse, NY

Other Available Reports

Other

Last Changed:	May 21, 2003
Order Number for Sorting:	
Remarks:	

2.6 WATER SOLUBILITY

Test Substance

Identity:	Hexadecanenitrile (CAS RN 629-79-8)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 310) WSKOWWIN Submodel (V 1.40)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: octanol-water partition coefficient, Log K_{ow} = 6.0.

Results

Value:	0.1132 mg/L
Solubility:	Soluble in water
pH value and concentration:	NA
pKa value at 25°C:	NA
Remarks:	Following are the results from the model:

```
Water Sol from Kow (WSKOW v1.40) Results:
=========================================

          Water Sol: 0.1132 mg/L

SMILES : C(#N)CCCCCCCCCCCCCCC
CHEM   : Hexadecanenitrile
MOL FOR: C16 H31 N1
MOL WT : 237.43
------------------------ WSKOW v1.40 Results -----------------
Log Kow  (estimated)  :  6.73
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  6.00 (user entered)

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
       (used when Melting Point NOT available)

      Correction(s):         Value
      -------------------   -----
       Nitrile              -0.265

   Log Water Solubility  (in moles/L) :  -6.322
   Water Solubility at 25 deg C (mg/L):  0.1132
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for WSKOW, version 1.3; Syracuse Research Corporation, North Syracuse, NY

Other Available Reports

Other

Last Changed:	May 21, 2003
Order Number for Sorting:	
Remarks:	

2.6 WATER SOLUBILITY

Test Substance

Identity:	Octadecanenitrile (CAS RN 638-65-3)
Purity:	Not stated
Remarks:	

Method

GLP:	Not stated
Year:	Not stated
Remarks:	

Results

Value:	Not stated
Solubility:	Insoluble
pH value and concentration:	Not stated
pKa value at 25°C:	Not stated
Remarks:	

Conclusions

Remarks:	The water solubility was provided in a reliable reference text (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions, endpoint provided in a reliable reference text.

References

Weast, R. C. and M. J. Astle, eds. 1980. CRC Handbook of Chemistry and Physics. CRC Press, Inc., Boca Raton, FL, U. S.

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	3
Remarks:	

2.6 WATER SOLUBILITY

Test Substance

Identity:	Nitriles, C16-18 (CAS RN 68002-65-3)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 310) WSKOWWIN Submodel (V 1.40)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Value:	0.009 mg/L
Solubility:	Soluble in water
pH value and concentration:	NA
pKa value at 25°C:	NA
Remarks:	Following are the results from the model:

```
Water Sol from Kow (WSKOW v1.40) Results:
=========================================

          Water Sol: 0.008592 mg/L

SMILES : C(#N)CCCCCCCCCCCCCCC
CHEM   : Nitriles, C16-18
MOL FOR: C17 H33 N1
MOL WT : 251.46
-------------------------- WSKOW v1.40 Results -------------------
Log Kow  (estimated)  :  7.22
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  7.22

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
       (used when Melting Point NOT available)

      Correction(s):         Value
      -------------------    -----
       Nitrile              -0.265

   Log Water Solubility  (in moles/L) :  -7.466
   Water Solubility at 25 deg C (mg/L):  0.008592
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for WSKOW, version 1.3; Syracuse Research Corporation, North Syracuse, NY

Other Available Reports

Other

Last Changed:	May 22, 2003
Order Number for Sorting:	
Remarks:	

2.6 WATER SOLUBILITY

Test Substance

Identity:	Nitriles, C16-22 (CAS RN 68153-02-6)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 310) WSKOWWIN Submodel (V 1.40)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Value:	0.0009 mg/L
Solubility:	Soluble in water
pH value and concentration:	NA
pKa value at 25°C:	NA
Remarks:	Following are the results from the model:

```
Water Sol from Kow (WSKOW v1.40) Results:
=========================================

          Water Sol: 0.000865 mg/L

SMILES : C(#N)CCCCCCCCCCCCCCCCC
CHEM   : Nitriles, C16-22
MOL FOR: C19 H37 N1
MOL WT : 279.51
--------------------------- WSKOW v1.40 Results ------------------
Log Kow  (estimated)  :  8.20
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  8.20

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
       (used when Melting Point NOT available)

      Correction(s):         Value
      -------------------    -----
       Nitrile              -0.265

   Log Water Solubility  (in moles/L) :  -8.509
   Water Solubility at 25 deg C (mg/L):  0.000865
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for WSKOW, version 1.3; Syracuse Research Corporation, North Syracuse, NY

Other Available Reports

Other

Last Changed:	May 23, 2003
Order Number for Sorting:	
Remarks:	

2.6 WATER SOLUBILITY

Test Substance

Identity:	Nitriles, C14-18 and C16-18, unsaturated (CAS RN 68513-04-2)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 310) WSKOWWIN Submodel (V 1.40)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Value:	0.10 mg/L
Solubility:	Soluble in water
pH value and concentration:	NA
pKa value at 25°C:	NA
Remarks:	Following are the results from the model:

```
Water Sol from Kow (WSKOW v1.40) Results:
=========================================

          Water Sol: 0.1034 mg/L

SMILES : C(#N)CC=CC=CCCCC=CCCCCC
CHEM   : Nitriles, C14-18 and C16-18-unsatd.
MOL FOR: C16 H25 N1
MOL WT : 231.38
--------------------------- WSKOW v1.40 Results ------------------
Log Kow  (estimated)  :  6.08
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  6.08

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
       (used when Melting Point NOT available)

      Correction(s):         Value
      -------------------    -----
       Nitrile              -0.265

   Log Water Solubility  (in moles/L) :  -6.350
   Water Solubility at 25 deg C (mg/L):  0.1034
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability: 2

Remarks: Reliable with restrictions; model data.

References Meylan W. and P.H. Howard. 1999. User's Guide for WSKOW, version 1.3; Syracuse Research Corporation, North Syracuse, NY

Other Available Reports

Other

Last Changed: May 23, 2003

Order Number for Sorting:

Remarks:

2.6 WATER SOLUBILITY

Test Substance

Identity:	Nitriles, C16 and C18 unsaturated (CAS RN 68002-64-2)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 310) WSKOWWIN Submodel (V 1.40)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Value:	0.007 mg/L
Solubility:	Soluble in water
pH value and concentration:	NA
pKa value at 25°C:	NA
Remarks:	Following are the results from the model:

```
Water Sol from Kow (WSKOW v1.40) Results:
=========================================

          Water Sol: 0.0067 mg/L

SMILES : C(#N)CCCCCCCC=CCC=CCCCCC
CHEM   : Nitriles, C16 and C18-unsatd.
MOL FOR: C18 H31 N1
MOL WT : 261.45
---------------------------- WSKOW v1.40 Results -----------------
Log Kow  (estimated)  :  7.28
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  7.28

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
       (used when Melting Point NOT available)

      Correction(s):         Value
      -------------------    -----
       Nitrile              -0.265

   Log Water Solubility  (in moles/L) :  -7.591
   Water Solubility at 25 deg C (mg/L):  0.0067
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

Meylan W. and P.H. Howard. 1999. User's Guide for WSKOW, version 1.3; Syracuse Research Corporation, North Syracuse, NY

Other Available Reports

Other

Last Changed:	May 23, 2003
Order Number for Sorting:	
Remarks:	

2.6 WATER SOLUBILITY

Test Substance

Identity:	Oleonitrile (CAS RN 112-91-4; 9-Octadecenenitrile)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Not stated
GLP:	Not stated
Year:	Not stated
Remarks:	

Results

Value:	Not stated
Solubility:	Insoluble
pH value and concentration:	Not stated
pKa value at 25°C:	Not stated
Remarks:	

Conclusions

Remarks:	The water solubility was provided in a reliable reference text (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions; endpoint provided in a reliable reference text.

References

Weast, R. C. and M. J. Astle, eds. 1980. CRC Handbook of Chemistry and Physics. CRC Press, Inc., Boca Raton, FL, U. S.

Other Available Reports

Other

Last Changed:	November 21, 2000
Order Number for Sorting:	1
Remarks:	

2.6 WATER SOLUBILITY

Test Substance

Identity:	Propionitrile, 3-(9-Octadecenylamino)- [CAS RN 26351-32-6; Propanenitrile, 3-(9-Octadecenylamino)-, (Z)-]
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 310) WSKOWWIN Submodel (V 1.40)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Value:	0.02 mg/L
Solubility:	Soluble in water
pH value and concentration:	NA
pKa value at 25°C:	NA
Remarks:	Following are the results from the model:

```
Water Sol from Kow (WSKOW v1.40) Results:
=========================================

          Water Sol: 0.02129 mg/L

SMILES : C(#N)CCNCCCCCCCCC=CCCCCCCCC
CHEM   : Propionitrile, 3-(9-octadecenylamino)-
MOL FOR: C21 H40 N2
MOL WT : 320.57
--------------------------- WSKOW v1.40 Results -----------------
Log Kow  (estimated)  :  7.47
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  7.47

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
       (used when Melting Point NOT available)

      Correction(s):         Value
      -------------------    -----
       Nitrile              -0.265
       Amine, aliphatic      1.008

   Log Water Solubility  (in moles/L) :  -7.178
   Water Solubility at 25 deg C (mg/L):  0.02129
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability: 2

Remarks: Reliable with restrictions; model data.

References Meylan W. and P.H. Howard. 1999. User's Guide for WSKOW, version 1.3; Syracuse Research Corporation, North Syracuse, NY

Other Available Reports

Other

Last Changed: May 26, 2003

Order Number for Sorting:

Remarks:

2.6 WATER SOLUBILITY

Test Substance

Identity:	Coco nitrile (CAS RN 61789-53-5; Nitriles, coco)
Purity:	No information provided
Remarks:	

Method

Method/Guideline followed:	No information provided
GLP:	Not stated
Year:	Not stated
Remarks:	

Results

Value:	Not stated
Solubility:	Practically insoluble
pH value and concentration:	No information provided
pKa value at 25°C:	No information provided
Remarks:	Information provided in reliable source

Conclusions

Remarks:	The water solubility was provided in a reliable reference text (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions; information provided in reliable source.

References

Jenkins, W. R. 1992. CESIO 40: Assessment of its ready biodegradability - Modified Sturm Test. Life Science Research Limited, Eye, Suffolk, UK.

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	6
Remarks:	

2.6 WATER SOLUBILITY

Test Substance

Identity:	Tallow-nitrile (CAS RN 61790-28-1; Nitriles, tallow)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Not stated
GLP:	Not stated
Year:	Not stated
Remarks:	

Results

Water Solubility:	Not soluble
Decomposition:	Not stated
Sublimation:	Not stated
Remarks:	

Conclusions

Remarks:	The water solubility was provided in a reliable reference text (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restriction; IUCLID summary of study conducted to guideline.

References Hoechst. 1992. Safety Data Sheet (19.06.1992). Cited in IUCLID (update 23-Oct-95).

Other Available Reports

Other

Last changed:	January 5, 2004
Order number for sorting:	37
Remarks:	

3.1.1 PHOTODEGRADATION

Test Substance

Identity:	Dodecanenitrile (CAS RN 2437-25-4)
Purity:	NA

Method

Method/guideline followed:	EPIWIN (v 3.10) AOPWIN submodel (v 1.90)
Type:	NA
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: octanol-water partition coefficient, Log K_{ow} = 4.9.

Results

Concentration of substance:	NA
Temperature °C:	NA
Direct photolysis:	NA
Indirect photolysis:	NA
	Breakdown products: NA
Remarks:	Overall OH Rate Constant (k_{phot}) = 11.6 E-12 cm^3/molecule-sec $t_{1/2}$ = 11.1 hours Following is the output from the model:

```
AOP Program (v1.90) Results:
============================
SMILES : C(#N)CCCCCCCCCC
CHEM   : Dodecanenitrile
MOL FOR: C12 H23 N1
MOL WT : 181.32
--------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ------------
Hydrogen Abstraction       =  11.5636 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =   0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant =  11.5636 E-12 cm3/molecule-sec
   HALF-LIFE =     0.925 Days (12-hr day; 1.5E6 OH/cm3)
   HALF-LIFE =    11.100 Hrs
---------- SUMMARY (AOP v1.90): OZONE REACTION -------------

           ******  NO OZONE REACTION ESTIMATION ******
           (ONLY Olefins and Acetylenes are Estimated)

Experimental Database:  NO Structure Matches
```

Conclusions

The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References

Meylan W. and P. H. Howard. 1999. User's Guide for AOPWIN, Version 1.9; Syracuse Research Corporation, North Syracuse, NY

Other

Last changed: May 21, 2003
Order number for sorting:
Remarks:

3.1.1 PHOTODEGRADATION

Test Substance

Identity:	Hexadecanenitrile (CAS RN 629-79-8)
Purity:	NA

Method

Method/guideline followed:	EPIWIN (v 3.10) AOPWIN submodel (v 1.90)
Type:	NA
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: octanol-water partition coefficient, Log K_{ow} = 6.0.

Results

Concentration of substance:	NA
Temperature °C:	NA
Direct photolysis:	NA
Indirect photolysis:	NA
Breakdown products:	NA
Remarks:	Overall OH Rate Constant ($k_{phot)}$ = 17 E-12 cm^3/molecule-sec $t_{1/2}$ = 7.46 days Following is the output from the model:

```
AOP Program (v1.90) Results:
============================
SMILES : C(#N)CCCCCCCCCCCCCC
CHEM   : Hexadecanenitrile
MOL FOR: C16 H31 N1
MOL WT : 237.43
------------ SUMMARY (AOP v1.90): HYDROXYL RADICALS ------------
Hydrogen Abstraction       =  17.2158 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =   0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant =  17.2158 E-12 cm3/molecule-sec
   HALF-LIFE =     0.621 Days (12-hr day; 1.5E6 OH/cm3)
   HALF-LIFE =     7.455 Hrs
------------ SUMMARY (AOP v1.90): OZONE REACTION --------------

               ******  NO OZONE REACTION ESTIMATION ******
               (ONLY Olefins and Acetylenes are Estimated)

Experimental Database:  NO Structure Matches
```

Conclusions

The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References

Meylan W. and P. H. Howard. 1999. User's Guide for AOPWIN, Version 1.9; Syracuse Research Corporation, North Syracuse, NY

Other

Last changed: May 21, 2003
Order number for sorting:
Remarks:

3.1.1 PHOTODEGRADATION

Test Substance

Identity:	Octadecanenitrile (CAS RN 638-65-3)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Calculated (Atkinson method)
Type:	Air
GLP:	No
Year:	1988
Light Source:	Not stated
Light Spectrum:	Not stated
Relative Intensity:	Not stated
Spectrum of Substance:	Not stated
Remarks:	

Results

Concentration of Substance:	Not stated
Temperature:	Not stated
Direct Photolysis:	Not stated
Oxygen radicals reaction:	Not stated
Ozone Reaction:	Not stated
Indirect Photolysis:	Degradation = 50% after 0.8 day
Breakdown products:	Not stated
Remarks:	Sensitizer = OH Concentration of sensitizer = 500,000 molecule/cm^3

Conclusions

Remarks:	The photodegradation of the test substance has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restriction; IUCLID summary of study conducted to guideline.

References

Hoechst. 1992. Einstufungsbegruendung TA-Luft der Abt. UCV (14.08.1992). Cited in IUCLID (update 23-Oct-95).

Remarks:

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	4a
Remarks:	

3.1.1 PHOTODEGRADATION

Test Substance

Identity:	Nitriles, C16-18 (CAS RN 68002-65-3)
Purity:	NA

Method

Method/guideline followed:	EPIWIN (v 3.10) AOPWIN submodel (v 1.90)
Type:	NA
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Concentration of substance:	NA
Temperature °C:	NA
Direct photolysis:	NA
Indirect photolysis:	NA
	Breakdown products: NA
Remarks:	Overall OH Rate Constant (k_{phot}) = 18.6 E-12 cm^3/molecule-sec $t_{1/2}$ = 6.89 hours Following is the output from the model:

```
AOP Program (v1.90) Results:
============================
SMILES : C(#N)CCCCCCCCCCCCCCC
CHEM   : Nitriles, C16-18
MOL FOR: C17 H33 N1
MOL WT : 251.46
---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS -----------
Hydrogen Abstraction       =  18.6288 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =   0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant =  18.6288 E-12 cm3/molecule-sec
   HALF-LIFE =     0.574 Days (12-hr day; 1.5E6 OH/cm3)
   HALF-LIFE =     6.890 Hrs

---------- SUMMARY (AOP v1.90): OZONE REACTION --------------

               ******  NO OZONE REACTION ESTIMATION ******
               (ONLY Olefins and Acetylenes are Estimated)

Experimental Database:  NO Structure Matches
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References Meylan W. and P. H. Howard. 1999. User's Guide for AOPWIN, Version 1.9; Syracuse Research Corporation, North Syracuse, NY

Other

Last changed: May 22, 2003
Order number for sorting:
Remarks:

3.1.1 PHOTODEGRADATION

Test Substance

Identity:	Nitriles, C16-22 (CAS RN 68153-02-6)
Purity:	NA

Method

Method/guideline followed:	EPIWIN (v 3.10) AOPWIN submodel (v 1.90)
Type:	NA
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Concentration of substance:	NA
Temperature °C:	NA
Direct photolysis:	NA
Indirect photolysis:	NA
	Breakdown products: NA
Remarks:	Overall OH Rate Constant (k_{phot}) = 21.5 E-12 cm^3/molecule-sec $t_{1/2}$ = 6.0 hours Following is the output from the model:

```
AOP Program (v1.90) Results:
============================
SMILES : C(#N)CCCCCCCCCCCCCCCCC
CHEM   : Nitriles, C16-22
MOL FOR: C19 H37 N1
MOL WT : 279.51
------------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ------------
Hydrogen Abstraction       =  21.4549 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =   0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant =  21.4549 E-12 cm3/molecule-sec
   HALF-LIFE =     0.499 Days (12-hr day; 1.5E6 OH/cm3)
   HALF-LIFE =     5.982 Hrs
------------- SUMMARY (AOP v1.90): OZONE REACTION --------------

               ******  NO OZONE REACTION ESTIMATION ******
               (ONLY Olefins and Acetylenes are Estimated)

Experimental Database:  NO Structure Matches
```

Conclusions

The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References

Meylan W. and P. H. Howard. 1999. User's Guide for AOPWIN, Version 1.9; Syracuse Research Corporation, North Syracuse, NY

Other

Last changed: May 23, 2003
Order number for sorting:
Remarks:

3.1.1 PHOTODEGRADATION

Test Substance

Identity:	Nitriles, C14-18 and C16-18, unsaturated (CAS RN 68513-04-2)
Purity:	NA

Method

Method/guideline followed:	EPIWIN (v 3.10) AOPWIN submodel (v 1.90)
Type:	NA
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Concentration of substance:	NA
Temperature °C:	NA
Direct photolysis:	NA
Indirect photolysis:	NA
	Breakdown products: NA
Remarks:	Overall OH Rate Constant ($k_{phot)}$ = 140 cm^3/molecule-sec $t_{1/2}$ = 0.92 hours The values were obtained by averaging the cis-isomer and trans-isomer values provided in the model. Following is the output from the model:

```
AOP Program (v1.90) Results:
============================
SMILES : C(#N)CC=CC=CCCCC=CCCCCC
CHEM   : Nitriles, C14-18 and C16-18-unsatd.
MOL FOR: C16 H25 N1
MOL WT : 231.38
---------------- SUMMARY (AOP v1.90): HYDROXYL RADICALS -------------------
Hydrogen Abstraction       =   9.1792 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
**Addition to Olefinic Bonds = 127.4000 E-12 cm3/molecule-sec [Cis-isomer]
**Addition to Olefinic Bonds = 135.0000 E-12 cm3/molecule-sec [Trans-isomer]
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant = 136.5792 E-12 cm3/molecule-sec [Cis-isomer]
   OVERALL OH Rate Constant = 144.1792 E-12 cm3/molecule-sec [Trans-isomer]
   HALF-LIFE =    0.940 Hrs (12-hr day; 1.5E6 OH/cm3) [Cis-isomer]
   HALF-LIFE =    0.890 Hrs (12-hr day; 1.5E6 OH/cm3) [Trans-isomer]
.....................  ** Designates Estimation(s) Using ASSUMED Value(s)
```

```
--------------- SUMMARY (AOP v1.90): OZONE REACTION ----------------------
   OVERALL OZONE Rate Constant =  45.000000 E-17 cm3/molecule-sec [Cis-]
   OVERALL OZONE Rate Constant =  52.000000 E-17 cm3/molecule-sec [Trans-]
   HALF-LIFE =  0.611 Hrs (at 7E11 mol/cm3) [Cis-isomer]
   HALF-LIFE =  0.529 Hrs (at 7E11 mol/cm3) [Trans-isomer]

 NOTE: Reaction with Nitrate Radicals May Be Important!

Experimental Database:  NO Structure Matches
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References Meylan W. and P. H. Howard. 1999. User's Guide for AOPWIN, Version 1.9; Syracuse Research Corporation, North Syracuse, NY

Other

Last changed: May 23, 2003
Order number for sorting:
Remarks:

3.1.1 PHOTODEGRADATION

Test Substance

Identity:	Nitriles, C16 and C18 unsaturated (CAS RN 68002-64-2)
Purity:	NA

Method

Method/guideline followed:	EPIWIN (v 3.10) AOPWIN submodel (v 1.90)
Type:	NA
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Concentration of substance:	NA
Temperature °C:	NA
Direct photolysis:	NA
Indirect photolysis:	NA
	Breakdown products: NA
Remarks:	Overall OH Rate Constant (k_{phot}) = 134 E-12 cm^3/molecule-sec $t_{1/2}$ = 0.96 hours The values were obtained by averaging the cis-isomer and trans-isomer values provided in the model. Following is the output from the model:

```
AOP Program (v1.90) Results:
============================
SMILES : C(#N)CCCCCCCC=CCC=CCCCCC
CHEM   : Nitriles, C16 and C18-unsatd.
MOL FOR: C18 H31 N1
MOL WT : 261.45
----------------- SUMMARY (AOP v1.90): HYDROXYL RADICALS -----------------
Hydrogen Abstraction       =  13.3822 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 112.8000 E-12 cm3/molecule-sec [Cis-isomer]
Addition to Olefinic Bonds = 128.0000 E-12 cm3/molecule-sec [Trans-isomer]
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant = 126.1822 E-12 cm3/molecule-sec [Cis-isomer]
   OVERALL OH Rate Constant = 141.3822 E-12 cm3/molecule-sec [Trans-isomer]
   HALF-LIFE =    1.017 Hrs (12-hr day; 1.5E6 OH/cm3) [Cis-isomer]
   HALF-LIFE =    0.908 Hrs (12-hr day; 1.5E6 OH/cm3) [Trans-isomer]
```

```
---------------- SUMMARY (AOP v1.90): OZONE REACTION --------------------
   OVERALL OZONE Rate Constant =  26.000000 E-17 cm3/molecule-sec [Cis-]
   OVERALL OZONE Rate Constant =  40.000000 E-17 cm3/molecule-sec [Trans-]
   HALF-LIFE =  1.058 Hrs (at 7E11 mol/cm3) [Cis-isomer]
   HALF-LIFE =  0.688 Hrs (at 7E11 mol/cm3) [Trans-isomer]

 NOTE: Reaction with Nitrate Radicals May Be Important!

Experimental Database:  NO Structure Matches
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References Meylan W. and P. H. Howard. 1999. User's Guide for AOPWIN, Version 1.9; Syracuse Research Corporation, North Syracuse, NY

Other

Last changed: May 23, 2003
Order number for sorting:
Remarks:

3.1.1 PHOTODEGRADATION

Test Substance

Identity:	9-Octadecenenitrile, (Z)- (CAS RN 112-91-4)
Purity:	NA

Method

Method/guideline followed:	EPIWIN (v 3.10) AOPWIN submodel (v 1.90)
Type:	NA
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: melting point = -1°C and boiling point = 330°C.

Results

Concentration of substance:	NA
Temperature °C:	NA
Direct photolysis:	NA
Indirect photolysis:	NA
	Breakdown products: NA
Remarks:	Overall OH Rate Constant (k_{phot}) = 77 E-12 cm^3/molecule-sec $t_{1/2}$ = 1.67 hours The values were obtained by averaging the cis-isomer and trans-isomer values provided in the model. Following is the output from the model:

```
AOP Program (v1.90) Results:
============================
SMILES : C(#N)CCCCCCCC=CCCCCCCCC
CHEM   : 9-Octadecenenitrile, (Z)-
MOL FOR: C18 H33 N1
MOL WT : 263.47
---------------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------------
Hydrogen Abstraction       =  16.6873 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =  56.4000 E-12 cm3/molecule-sec [Cis-isomer]
Addition to Olefinic Bonds =  64.0000 E-12 cm3/molecule-sec [Trans-isomer]
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant =  73.0873 E-12 cm3/molecule-sec [Cis-isomer]
   OVERALL OH Rate Constant =  80.6873 E-12 cm3/molecule-sec [Trans-isomer]
   HALF-LIFE =    1.756 Hrs (12-hr day; 1.5E6 OH/cm3) [Cis-isomer]
   HALF-LIFE =    1.591 Hrs (12-hr day; 1.5E6 OH/cm3) [Trans-isomer]
```

```
---------------- SUMMARY (AOP v1.90): OZONE REACTION --------------------
   OVERALL OZONE Rate Constant =  13.000000 E-17 cm3/molecule-sec [Cis-]
   OVERALL OZONE Rate Constant =  20.000000 E-17 cm3/molecule-sec [Trans-]
   HALF-LIFE =  2.116 Hrs (at 7E11 mol/cm3) [Cis-isomer]
   HALF-LIFE =  1.375 Hrs (at 7E11 mol/cm3) [Trans-isomer]

 NOTE: Reaction with Nitrate Radicals May Be Important!

Experimental Database:  NO Structure Matches
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References Meylan W. and P. H. Howard. 1999. User's Guide for AOPWIN, Version 1.9; Syracuse Research Corporation, North Syracuse, NY

Other

Last changed: May 23, 2003
Order number for sorting:
Remarks:

3.1.1 PHOTODEGRADATION

Test Substance

Identity:	Propionitrile, 3-(9-Octadecenylamino)- [CAS RN 26351-32-6; Propanenitrile, 3-(9-Octadecenylamino)-, (Z)-]
Purity:	NA

Method

Method/guideline followed:	EPIWIN (v 3.10) AOPWIN submodel (v 1.90)
Type:	NA
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Concentration of substance:	NA
Temperature °C:	NA
Direct photolysis:	NA
Indirect photolysis:	NA
	Breakdown products: NA
Remarks:	Overall OH Rate Constant ($k_{phot)}$ = 91.3 E-12 cm^3/molecule-sec $t_{1/2}$ = 1.41 hours The values were obtained by averaging the cis-isomer and trans-isomer values provided in the model. Following is the output from the model:

```
AOP Program (v1.90) Results:
============================
SMILES : C(#N)CCNCCCCCCCCC=CCCCCCCCC
CHEM   : Propionitrile, 3-(9-octadecenylamino)-
MOL FOR: C21 H40 N2
MOL WT : 320.57
---------------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------------
Hydrogen Abstraction       =  31.1019 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =  56.4000 E-12 cm3/molecule-sec [Cis-isomer]
Addition to Olefinic Bonds =  64.0000 E-12 cm3/molecule-sec [Trans-isomer]
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant =  87.5019 E-12 cm3/molecule-sec [Cis-isomer]
   OVERALL OH Rate Constant =  95.1019 E-12 cm3/molecule-sec [Trans-isomer]
   HALF-LIFE =    1.467 Hrs (12-hr day; 1.5E6 OH/cm3) [Cis-isomer]
   HALF-LIFE =    1.350 Hrs (12-hr day; 1.5E6 OH/cm3) [Trans-isomer]
```

```
---------------- SUMMARY (AOP v1.90): OZONE REACTION --------------------
   OVERALL OZONE Rate Constant =  13.000000 E-17 cm3/molecule-sec [Cis-]
   OVERALL OZONE Rate Constant =  20.000000 E-17 cm3/molecule-sec [Trans-]
   HALF-LIFE =  2.116 Hrs (at 7E11 mol/cm3) [Cis-isomer]
   HALF-LIFE =  1.375 Hrs (at 7E11 mol/cm3) [Trans-isomer]

 NOTE: Reaction with Nitrate Radicals May Be Important!

Experimental Database:  NO Structure Matches
```

Conclusions The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References Meylan W. and P. H. Howard. 1999. User's Guide for AOPWIN, Version 1.9; Syracuse Research Corporation, North Syracuse, NY

Other

Last changed: May 26, 2003
Order number for sorting:
Remarks:

3.1.1 PHOTODEGRADATION

Test Substance

Identity:	Tallow - nitrile (CAS RN 61790-28-1; Nitriles, tallow)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Calculated (Atkinson method)
Type:	Air
GLP:	Not stated
Year:	1988
Light Source:	Not stated
Light Spectrum:	Not stated
Relative Intensity:	Not stated
Spectrum of Substance:	Not stated
Remarks:	

Results

Concentration of Substance:	Not stated
Temperature:	Not stated
Direct Photolysis:	Not stated
Oxygen radicals reaction:	Not stated
Ozone Reaction:	Not stated
Indirect Photolysis:	Degradation: C_{12} = approximately 50% after 1.4 days C_{20} = approximately 50% after 0.7 day
Breakdown products:	Not stated
Remarks:	Sensitizer = OH Concentration of sensitizer = 500,000 molecule/cm^3

Conclusions

Remarks:	The photodegradation of the test substance has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restriction; IUCLID summary of study conducted to guideline.

References Hoechst. 1992. Selbsteinstufung TA Luft der Abt. UCV (14.08.1992). Cited in IUCLID (update 23-Oct-95).

Remarks:

Other Available Reports

Other

Last Changed: January 5, 2004
Order Number for Sorting: 37
Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity:	Dodecanenitrile (CAS RN 2437-25-4)
Purity:	NA

Method

Method/Guideline followed:	Equilibrium Concentration Model (EQC) Level III (V 1.01) Calculation according to Mackay, Level III
Media:	Water, air, soil and sediment (model run with emissions to water = 1000 kg/hr and emissions to air, soil and sediment = 0 kg/hr each)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run using the following physical chemical properties: octanol-water partition coefficient, Log K_{ow} = 4.9.

Results

Remarks: Following are the results from the model:

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : Dodecanenitrile
  Molecular Wt: 181.32
  Henry's LC  : 0.000848 atm-m3/mole (Henrywin program)
  Vapor Press : 0.00628 mm Hg  (Mpbpwin program)
  Log Kow     : 4.9  (user-entered)
  Soil Koc    : 3.26e+004  (calc by model)

           Mass Amount    Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       2.98            22.2         0
   Water     66.8            360          1000
   Soil      0.038           360          0
   Sediment  30.2            1.44e+003    0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       1.2e-011     279         89.3        27.9        8.93
   Water     4.45e-009    386         200         38.6        20
   Soil      3.79e-014    0.22        0           0.022       0
   Sediment  1.35e-009    43.5        1.81        4.35        0.181

   Persistence Time: 300 hr
   Reaction Time:    423 hr
   Advection Time:   1.03e+003 hr
   Percent Reacted:  70.8
   Percent Advected: 29.2

   Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
```

```
            Air:      22.2
            Water:    360
            Soil:     360
            Sediment: 1440
              Biowin estimate: 3.014  (weeks       )

         Advection Times (hr):
            Air:      100
            Water:    1000
            Sediment: 5e+004
```

Conclusions

Mass Amount (percent):
Air: 3.0%
Water: 66.8%
Soil: < 1%
Sediment: 30.2%

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References

Mackay, D., A. DiGuardo, S. Paterson and C. E. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ. Toxicol. Chem. 15(9): 1627-1637

Other

Last changed: May 21, 2003
Order number for sorting:
Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity:	Hexadecanenitrile (CAS RN 629-79-8)
Purity:	NA

Method

Method/Guideline followed:	Equilibrium Concentration Model (EQC) Level III (V 1.01) Calculation according to Mackay, Level III
Media:	Water, air, soil and sediment (model run with emissions to water = 1000 kg/hr and emissions to air, soil and sediment = 0 kg/hr each)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run using the following physical chemical properties: octanol-water partition coefficient, Log K_{ow} = 6.0.

Results

Remarks: Following are the results from the model:

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : Hexadecanenitrile
  Molecular Wt: 237.43
  Henry's LC  : 0.00338 atm-m3/mole (Henrywin program)
  Vapor Press : 0.00246 mm Hg  (Mpbpwin program)
  Liquid VP   : 0.00713 mm Hg  (super-cooled)
  Melting Pt  : 71.7 deg C (Mpbpwin program)
  Log Kow     : 6  (user-entered)
  Soil Koc    : 4.1e+005  (calc by model)

            Mass Amount    Half-Life    Emissions
             (percent)        (hr)       (kg/hr)
   Air       0.542           14.9         0
   Water     21.9            360          1000
   Soil      0.0062          360          0
   Sediment  77.6            1.44e+003    0

              Fugacity    Reaction    Advection   Reaction    Advection
               (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       4.18e-012    189         40.6         18.9         4.06
   Water     7.01e-009    315         164          31.5         16.4
   Soil      3.73e-015    0.0894      0            0.00894      0
   Sediment  2.1e-009     280         11.6         28           1.16

   Persistence Time: 749 hr
   Reaction Time:    956 hr
   Advection Time:   3.47e+003 hr
   Percent Reacted:  78.4
   Percent Advected: 21.6
```

```
Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      14.91
   Water:    360
   Soil:     360
   Sediment: 1440
     Biowin estimate: 2.890  (weeks       )

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Conclusions

Mass Amount:
Air: < 1%
Water: 21.9%
Soil: < 1%
Sediment:77.6%

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References

Mackay, D., A. DiGuardo, S. Paterson and C. E. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ. Toxicol. Chem. 15(9): 1627-1637

Other

Last changed: May 21, 2003
Order number for sorting:
Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity:	Octadecanenitrile (CAS RN 638-65-3)
Purity:	NA

Method

Method/Guideline followed:	Equilibrium Concentration Model (EQC) Level III (V 1.01) Calculation according to Mackay, Level III
Media:	Water, air, soil and sediment (model run with emissions to water = 1000 kg/hr and emissions to air, soil and sediment = 0 kg/hr each)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: melting point = 41°C; boiling point = 362°C; octanol-water partition coefficient, Log K_{ow} = 6.0.

Results

Remarks: Following are the results from the model:

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : Octadecanenitrile
  Molecular Wt: 265.49
  Henry's LC  : 0.00674 atm-m3/mole (Henrywin program)
  Vapor Press : 0.000102 mm Hg  (Mpbpwin program)
  Liquid VP   : 0.000146 mm Hg  (super-cooled)
  Melting Pt  : 41 deg C (user-entered)
  Log Kow     : 6  (user-entered)
  Soil Koc    : 4.1e+005  (calc by model)

           Mass Amount    Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       0.493           12.8         0
   Water     21.9            360          1000
   Soil      0.0469          360          0
   Sediment  77.6            1.44e+003    0

             Fugacity    Reaction   Advection   Reaction   Advection
             (atm)      (kg/hr)     (kg/hr)    (percent)   (percent)
   Air       3.35e-012    198        36.6        19.8        3.66
   Water     1.24e-008    313        163         31.3        16.3
   Soil      4.99e-014    0.671      0           0.0671      0
   Sediment  3.72e-009    278        11.5        27.8        1.15
```

```
Persistence Time: 743 hr
Reaction Time:    942 hr
Advection Time:   3.53e+003 hr
Percent Reacted:  78.9
Percent Advected: 21.1

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      12.81
   Water:    360
   Soil:     360
   Sediment: 1440
     Biowin estimate: 2.828  (weeks       )

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Conclusions

Mass Amount:
Air: < 1%
Water: 21.9%
Soil: < 1%
Sediment: 77.6%

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References

Mackay, D., A. DiGuardo, S. Paterson and C. E. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ. Toxicol. Chem. 15(9): 1627-1637

Other

Last changed: May 22, 2003
Order number for sorting:
Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity:	Nitriles, C16-18 (CAS RN 68002-65-3)
Purity:	NA

Method

Method/Guideline followed:	Equilibrium Concentration Model (EQC) Level III (V 1.01) Calculation according to Mackay, Level III
Media:	Water, air, soil and sediment (model run with emissions to water = 1000 kg/hr and emissions to air, soil and sediment = 0 kg/hr each)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Remarks: Following are the results from the model:

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : Nitriles, C16-18
  Molecular Wt: 251.46
  Henry's LC  : 0.00477 atm-m3/mole (Henrywin program)
  Vapor Press : 0.00147 mm Hg  (Mpbpwin program)
  Liquid VP   : 0.00526 mm Hg  (super-cooled)
  Melting Pt  : 80.8 deg C (Mpbpwin program)
  Log Kow     : 7.22  (Kowwin program)
  Soil Koc    : 6.8e+006  (calc by model)

            Mass Amount    Half-Life    Emissions
             (percent)        (hr)       (kg/hr)
   Air       0.0358          13.8         0
   Water     10.9            360          1000
   Soil      0.000429        360          0
   Sediment  89              1.44e+003    0

              Fugacity    Reaction    Advection   Reaction
Advection
               (atm)      (kg/hr)      (kg/hr)    (percent)
(percent)
   Air       4.42e-013    22.9        4.55        2.29        0.455
   Water     1.09e-009    267         139         26.7        13.9
   Soil      3.51e-017    0.0105      0           0.00105     0
   Sediment  3.28e-010    544         22.6        54.4        2.26
```

```
Persistence Time: 1.27e+003 hr
Reaction Time:    1.52e+003 hr
Advection Time:   7.64e+003 hr
Percent Reacted:  83.4
Percent Advected: 16.6

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      13.78
   Water:    360
   Soil:     360
   Sediment: 1440
     Biowin estimate: 2.859  (weeks       )

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Conclusions

Mass Amount:
Air: < 1%
Water: 10.9%
Soil: < 1%
Sediment: 89%

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References

Mackay, D., A. DiGuardo, S. Paterson and C. E. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ. Toxicol. Chem. 15(9): 1627-1637

Other

Last changed: May 22, 2003
Order number for sorting:
Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity:	Nitriles, C16-22 (CAS RN 68153-02-6)
Purity:	NA

Method

Method/Guideline followed:	Equilibrium Concentration Model (EQC) Level III (V 1.01) Calculation according to Mackay, Level III
Media:	Water, air, soil and sediment (model run with emissions to water = 1000 kg/hr and emissions to air, soil and sediment = 0 kg/hr each)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Remarks: Following are the results from the model:

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : Nitriles, C16-22
  Molecular Wt: 279.51
  Henry's LC  : 0.00952 atm-m3/mole (Henrywin program)
  Vapor Press : 0.000252 mm Hg  (Mpbpwin program)
  Liquid VP   : 0.00136 mm Hg  (super-cooled)
  Melting Pt  : 98.9 deg C (Mpbpwin program)
  Log Kow     : 8.2  (Kowwin program)
  Soil Koc    : 6.5e+007  (calc by model)

            Mass Amount    Half-Life    Emissions
             (percent)        (hr)       (kg/hr)
   Air       0.00344         12           0
   Water     10.2            360          1000
   Soil      6.45e-005       360          0
   Sediment  89.8            1.44e+003    0

              Fugacity    Reaction    Advection   Reaction
Advection
               (atm)      (kg/hr)      (kg/hr)    (percent)
(percent)
   Air       4e-014       2.66        0.458       0.266       0.0458
   Water     2.18e-010    262         136         26.2        13.6
   Soil      1.04e-018    0.00165     0           0.000165    0
   Sediment  6.53e-011    575         23.9        57.5        2.39

   Persistence Time: 1.33e+003 hr
   Reaction Time:    1.59e+003 hr
   Advection Time:   8.3e+003 hr
```

```
Percent Reacted:  84
Percent Advected: 16

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      11.96
   Water:    360
   Soil:     360
   Sediment: 1440
     Biowin estimate: 2.797  (weeks       )

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Conclusions

Mass Amount:
Air: < 1%
Water: 10.2%
Soil: < 1%
Sediment: 89.8%

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data

References

Mackay, D., A. DiGuardo, S. Paterson and C. E. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ. Toxicol. Chem. 15(9): 1627-1637

Other

Last changed: May 23, 2003

Order number for sorting:

Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity:	Nitriles, C14-18 and C16-18, unsaturated (CAS RN 68513-04-2)
Purity:	NA

Method

Method/Guideline followed:	Equilibrium Concentration Model (EQC) Level III (V 1.01) Calculation according to Mackay, Level III
Media:	Water, air, soil and sediment (model run with emissions to water = 1000 kg/hr and emissions to air, soil and sediment = 0 kg/hr each)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Remarks: Following are the results from the model:

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : Nitriles, C14-18 and C16-18-unsatd.
  Molecular Wt: 231.38
  Henry's LC  : 0.000894 atm-m3/mole (Henrywin program)
  Vapor Press : 0.00037 mm Hg  (Mpbpwin program)
  Liquid VP   : 0.000768 mm Hg  (super-cooled)
  Melting Pt  : 57 deg C (Mpbpwin program)
  Log Kow     : 6.08  (Kowwin program)
  Soil Koc    : 4.93e+005  (calc by model)

            Mass Amount    Half-Life    Emissions
             (percent)        (hr)       (kg/hr)
   Air       0.0146          0.461        0
   Water     20.2            360          1000
   Soil      0.000396        360          0
   Sediment  79.8            1.44e+003    0

              Fugacity    Reaction    Advection   Reaction    Advection
               (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       1.27e-013    181          1.2         18.1        0.12
   Water     1.79e-009    321          167         32.1        16.7
   Soil      5.92e-017    0.00628      0           0.000628    0
   Sediment  5.37e-010    317          13.2        31.7        1.32

   Persistence Time: 825 hr
   Reaction Time:    1.01e+003 hr
   Advection Time:   4.55e+003 hr
   Percent Reacted:  81.9
```

```
Percent Advected: 18.1

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      0.4613
   Water:    360
   Soil:     360
   Sediment: 1440
     Biowin estimate: 2.904  (weeks       )

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Conclusions

Mass Amount:
Air: < 1%
Water: 20.2%
Soil: < 1%
Sediment: 79.8%

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References

Mackay, D., A. DiGuardo, S. Paterson and C. E. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ. Toxicol. Chem. 15(9): 1627-1637

Other

Last changed: May 23, 2003
Order number for sorting:
Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity:	Nitriles, C16 and C18 unsaturated (CAS RN 68002-64-2)
Purity:	NA

Method

Method/Guideline followed:	Equilibrium Concentration Model (EQC) Level III (V 1.01) Calculation according to Mackay, Level III
Media:	Water, air, soil and sediment (model run with emissions to water = 1000 kg/hr and emissions to air, soil and sediment = 0 kg/hr each)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Remarks: Following are the results from the model:

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : Nitriles, C16 and C18-unsatd.
  Molecular Wt: 261.45
  Henry's LC  : 0.000466 atm-m3/mole (Henrywin program)
  Vapor Press : 0.000248 mm Hg  (Mpbpwin program)
  Liquid VP   : 0.00101 mm Hg  (super-cooled)
  Melting Pt  : 86.8 deg C (Mpbpwin program)
  Log Kow     : 7.28  (Kowwin program)
  Soil Koc    : 7.81e+006  (calc by model)

            Mass Amount    Half-Life    Emissions
             (percent)        (hr)       (kg/hr)
   Air       0.00129         0.696        0
   Water     10.8            360          1000
   Soil      3.16e-005       360          0
   Sediment  89.2            1.44e+003    0

              Fugacity    Reaction    Advection   Reaction    Advection
               (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       1.55e-014    16.6         0.166       1.66        0.0166
   Water     9.1e-011     269          140         26.9        14
   Soil      2.15e-019    0.000783     0           7.83e-005   0
   Sediment  2.73e-011    552          22.9        55.2        2.29

   Persistence Time: 1.29e+003 hr
   Reaction Time:    1.54e+003 hr
   Advection Time:   7.91e+003 hr
   Percent Reacted:  83.7
   Percent Advected: 16.3
```

```
Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      0.696
   Water:    360
   Soil:     360
   Sediment: 1440
     Biowin estimate: 2.837  (weeks       )

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Conclusions

Mass Amount:
Air: < 1%
Water: 10.8%
Soil: < 1%
Sediment: 89.2%

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References

Mackay, D., A. DiGuardo, S. Paterson and C. E. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ. Toxicol. Chem. 15(9): 1627-1637

Other

Last changed: May 23, 2003
Order number for sorting:
Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity:	9-Octadecenenitrile, (Z)- (CAS RN 112-91-4)
Purity:	NA

Method

Method/Guideline followed:	Equilibrium Concentration Model (EQC) Level III (V 1.01) Calculation according to Mackay, Level III
Media:	Water, air, soil and sediment (model run with emissions to water = 1000 kg/hr and emissions to air, soil and sediment = 0 kg/hr each)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: melting point = -1°C and boiling point = 330°C.

Results

Remarks: Following are the results from the model:

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : 9-Octadecenenitrile, (Z)-
  Molecular Wt: 263.47
  Henry's LC  : 0.00177 atm-m3/mole (Henrywin program)
  Vapor Press : 0.000391 mm Hg  (Mpbpwin program)
  Log Kow     : 7.5  (Kowwin program)
  Soil Koc    : 1.3e+007  (calc by model)

           Mass Amount    Half-Life    Emissions
            (percent)       (hr)       (kg/hr)
   Air       0.00197         1.32         0
   Water     10.6            360          1000
   Soil      8.31e-005       360          0
   Sediment  89.4            1.44e+003    0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       2.37e-014    13.5        0.256       1.35        0.0256
   Water     2.1e-010     265         138         26.5        13.8
   Soil      1.3e-018     0.00208     0           0.000208    0
   Sediment  6.29e-011    561         23.3        56.1        2.33

   Persistence Time: 1.3e+003 hr
   Reaction Time:    1.55e+003 hr
   Advection Time:   8.08e+003 hr
   Percent Reacted:  83.9
   Percent Advected: 16.1
```

```
Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      1.32
   Water:    360
   Soil:     360
   Sediment: 1440
     Biowin estimate: 2.833  (weeks       )

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Conclusions

Mass Amount:
Air: < 1%
Water: 10.6%
Soil: < 1%
Sediment: 89.4%

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References

Mackay, D., A. DiGuardo, S. Paterson and C. E. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ. Toxicol. Chem. 15(9): 1627-1637

Other

Last changed: May 23, 2003
Order number for sorting:
Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity:	Propionitrile, 3-(9-Octadecenylamino)- [CAS RN 26351-32-6; Propanenitrile, 3-(9-Octadecenylamino)-, (Z)-]
Purity:	NA

Method

Method/Guideline followed:	Equilibrium Concentration Model (EQC) Level III (V 1.01) Calculation according to Mackay, Level III
Media:	Water, air, soil and sediment (model run with emissions to water = 1000 kg/hr and emissions to air, soil and sediment = 0 kg/hr each)
GLP:	NA
Year:	2003
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Remarks: Following are the results from the model:

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : Propionitrile, 3-(9-octadecenylamino)-
  Molecular Wt: 320.57
  Henry's LC  : 1.54e-007 atm-m3/mole (Henrywin program)
  Vapor Press : 4.65e-005 mm Hg  (Mpbpwin program)
  Liquid VP   : 0.000767 mm Hg  (super-cooled)
  Melting Pt  : 148 deg C (Mpbpwin program)
  Log Kow     : 7.47  (Kowwin program)
  Soil Koc    : 1.21e+007  (calc by model)

            Mass Amount    Half-Life    Emissions
             (percent)        (hr)       (kg/hr)
   Air       6.48e-007       1.23         0
   Water     5.02            900          1000
   Soil      1.29e-005       900          0
   Sediment  95              3.6e+003     0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       1.7e-017     0.0126      0.000223    0.00126     2.23e-005
   Water     2.01e-014    133         173         13.3        17.3
   Soil      4.09e-023    0.000343    0           3.43e-005   0
   Sediment  1.35e-014    629         65.4        62.9        6.54

   Persistence Time: 3.44e+003 hr
   Reaction Time:    4.51e+003 hr
   Advection Time:   1.45e+004 hr
```

```
Percent Reacted:  76.2
Percent Advected: 23.8

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      1.229
   Water:    900
   Soil:     900
   Sediment: 3600
     Biowin estimate: 2.731  (weeks-months)

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Conclusions

Mass Amount:
Air: < 1%
Water: 5.0%
Soil: < 1%
Sediment: 95.0%

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References

Mackay, D., A. DiGuardo, S. Paterson and C. E. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ. Toxicol. Chem. 15(9): 1627-1637

Other

Last changed: May 26, 2003
Order number for sorting:
Remarks:

3.5 BIODEGRADATION

Test Substance

Identity:	Dodecanenitrile (CAS RN 2437-25-4)
Purity:	Not stated.
Remarks:	

Method

Method/Guideline followed:	Directive 84/449/EEC, C.7 "Biotic degradation – modified MITI test"
Test Type:	Aerobic
GLP:	No
Year:	1987
Contact Time:	28 days
Inoculum:	Activated sludge, domestic
Remarks:	

Results

Degradation:	15%
Results:	Not stated
Kinetic:	Not stated
Breakdown Products:	Not stated
Remarks:	

Conclusions

Remarks:	The biodegradability of the test substance was adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restriction; IUCLID summary of study conducted to guideline.

References Hoechst. 1987. Unpublished document (W87-680). Cited in IUCLID (update 23-Oct-95).

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	5
Remarks:	

3.5 BIODEGRADATION

Test Substance

Identity:	CESIO 40 (CAS RN 61789-53-5; Nitriles, coco)
Purity:	Purity provided as percent distribution of carbon chain lengths from C8 to C18.
Remarks:	

Method

Method/Guideline followed:	OECD Guidelines for Testing of Chemicals, Guideline 301B and EEC Procedure C5
Test Type:	CO_2 evolution – Modified Sturm Test
GLP:	Yes
Year:	1992
Contact Time:	28 days
Inoculum:	Activated sludge supernatant at 1% v/v.
Remarks:	Four vessels were prepared to contain 3.5 liters of mineral salts medium. To one vessel only inoculum was added, to a second vessel, inoculum with sodium benzoate at 20 mg/l was added, to a third vessel, inoculum with test substance at 10 mg/l was added and to the fourth vessel, inoculum with test substance at 20 mg/l was added. Following preparation of the test vessels, 500 ml of solution was removed from each vessel for the determination of pH and DOC. Each vessel then was fitted with an air inlet tube reaching 15 cm below the surface of the liquid and outlet tube connected to three Drechsel bottles in series, each containing 100 ml 0.025 N barium hydroxide. The vessels were continuously flushed with CO_2-free air for 27 days. Periodically, one Drechsel bottle closest to the test vessel was removed and titrated for CO_2 content. A fresh Drechsel bottle was added at the end. On day 27, concentrated hydrochloric acid was added to the test vessels to drive off inorganic CO_2 and the vessels were aerated overnight. Final titrations were done on day 28. At the start and end of the test, test and control samples were removed and analyzed for DOC. Temperatures in the test area ranged from 18.6 to 21.6 °C during the test.

Results

Degradation:	Cumulative CO_2 production of solutions containing the test substance at 10 and 20 mg/l was equivalent to 25% and 43% of the theoretical CO_2 content.
Results:	Degradation achieved 25% and 43% of the ThCO_2 by day 28, indicating that the test substance was not readily biodegradable under the conditions of the test.

Kinetic:	No information provided
Breakdown Products:	No information provided
Remarks:	A preliminary 5-day bacterial inhibition assay conducted at 2 and 10 mg/l showed that the test substance was not inhibitory to the inoculum. Carbon analysis at the beginning and end of the test (DOC) indicated that the test substance was not in solution so degradation based on DOC removal could not be calculated.

Conclusions

Remarks:	The ready biodegradability of the test substance in the Modified Sturm Test was adequately characterized by the study (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study (OECD)

References

Jenkins, W. R. 1992. CESIO 40: Assessment of its ready biodegradability, Modified Sturm Test. Confidential report number 92/CFY003/0108. Life Science Research Limited, Eye, Suffolk, UK.

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	6
Remarks:	

3.5 BIODEGRADATION

Test Substance

Identity:	Arneel C (CAS RN 61789-53-5; Nitriles, coco)
Purity:	Approximately 100%
Remarks:	

Method

Method/Guideline followed:	OECD Guideline 301B, CO_2 Evolution Test
Test type:	Aerobic ready biodegradability
GLP:	Yes
Year:	1996
Contact time:	28 days
Inoculum:	Activated sludge
Remarks:	The ready biodegradability in the Modified Sturm Test was determined with the nonadapted activated sludge for the test substance over a period of 28 days. The test vessels contained approximately 18×10^2 colony forming units/ml of inoculum. The test substance was tested in a concentration of 13 mg/l in duplicates, corresponding to a carbon content of 10.4 mg C/l. The biological degradation of the test substance was followed by titrimetric analyses of the quantity of CO_2, which was produced by the respiration of bacteria. The degradation was terminated on day 28 with HCl and the last titration was made on day 29, after the soluble CO_2 was turned out over a period of 24 hours. The CO_2 production was calculated as the percentage of total CO_2 that the test substance could have theoretically produced based on carbon composition. Biodegradability was, therefore, expressed as a percentage $ThCO_2$ and was calculated for each titration of CO_2. In order to check the activity of the study system, sodium acetate (35 mg/l, single replicate) was used as the functional control. A negative control comprising nutrient solution and inoculum (duplicate) and a toxicity control comprising the test substance (13 mg/l) and the functional control (35 mg/l) also were tested (single replicate). The following deviations from the guideline occurred: 1) The guideline recommends the range of colony forming units between 10^6-10^8 colony forming units/ml. A bacterial density was chosen which, from experience, quickly adapted for the biodegradation of the ready biodegradable functional control. Also, the test duration of 28 days allows sufficient time for adaptation of the microorganisms to the test compounds. 2) The relation between IC and TC content of the test substance in the mineral medium was not

determined at the beginning of the test because the test substance was not fully soluble in the test medium.

Results

Degradation:	The pass level of 10% (start of the degradation phase) was reached by the test substance at the fourth day. In the 10-day window the test substance came to a mean degradation rate of 59%. After 28 days a mean degradation rate of 71% was reached. The test substance was considered readily biodegradable under the conditions of this test.
Results:	27.1 mg/l $C0_2$ production after 28 days: $ThCO_2$ = 38.2 mg/l.
Kinetic:	Degradation of test substance over time: 6 days = 24% 13 days = 59% 20 days = 65% 28 days = 71%
Breakdown products:	Not stated
Remarks:	The functional control was degraded to 72% after 13 days and, therefore, the quality criterion of "degradation > 60% after 14 days" was fulfilled. In the toxicity control the degradation came to a rate of 57% after 13 days and reached a maximum of 63% after 28 days, fulfilling the guideline criterion of "degradation > 25% after 14 days". The temperatures in the water bath during incubation times ranged from 23 to 24 °C.

Conclusions

Remarks:	The test substance must be regarded as readily biodegradable (Author of report). The biodegradation of Coconitrile has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Noack, M. 1996. Arneel C ready biodegradability Modified Sturm Test. Study number AST49091. Dr. U. Noack-Laboratorium, Hildesheim, Germany.

Other

Last changed:	April 17, 2001
Order number for sorting:	20b
Remarks:	

3.5 BIODEGRADATION

Test Substance

Identity:	FARNIL TH-D (CAS RN 61790-29-2; Nitriles, tallow, hydrogenated)
Purity:	100% Technical grade
Remarks:	

Method

Method/Guideline followed:	OECD Guideline 301F, Ready Biodegradability: Manometric Respirometry Test, Directive 92/69 EEC, C.4-D and DIN 38409, H-41
Test type:	Aerobic ready biodegradability
GLP:	Yes
Year:	1995
Contact time:	28 days
Inoculum:	Activated sludge
Remarks:	The test substance was tested for its biodegradability in the Manometric Respirometry Test by exposing it to microorganisms from the secondary effluent of a domestic waste water treatment plant for a period of 28 days. The concentration of the test substance in the test medium was approximately 100 mg/l. Duplicate flasks containing the test substance were tested. As a reference compound, Aniline was tested simultaneously under the same conditions at a concentration of approximately 100 mg/l. The test substance also was tested in the test medium, but with no inoculum (abiotic control), and with Aniline, test medium and inoculum (toxicity control). No emulsifiers or solvents were used, but ultrasonic dispersion was employed to achieve a good dispersion of the test substance. The chemical oxygen demand (COD) was determined in each flasks. The COD was validated with two positive (potassium hydrogenphtalate solution) and two blank (water) controls. The COD determination was considered valid if no more than 10% of the oxidizing agent was used up in the blank control and if the COD of the positive control was between 192 and 208 mg/l. Due to technical problems, the study was terminated after 26 rather than 28 days but the test was considered adequate to fulfill the Guideline requirements.

Results

Degradation:	The biochemical oxygen demand in the two test flasks containing inoculum and the test substance at a concentration of approximately 25 mg/l reached 10% of the COD on about exposure day 5. At the end of the 10-day

window on exposure day 15, average degradation was 78.2% of COD; therefore, the pass level for ready biodegradability was reached. At the end of the test an average degradation rate of 110.1% of COD was obtained. The reference compound, Aniline, was biodegraded by 60% of ThOD on exposure day 14, and by 65% at the end of the 10-day window on exposure day 18. At the end of the test, Aniline was biodegraded by 71.9% of ThOD. In the toxicity control, no inhibitory effect on the microorganisms was observed. The pH after 26 days of exposure was 7.4. The test substance was considered readily biodegradable under the conditions of this test. Although the test was terminated at 26 days, the results are reported for 28 days since all of the test substance degraded and the Guideline specifies 28 days.

Results: Mean COD of the test substance was 195.2 mg O_2/100mg

Kinetic: Degradation of test substance over time:
Day 5 = 7.7%
Day 10 = 48.4%
Day 15 = 78.2%
Day 20 = 96.2%
Day 26 = 110.1%

Breakdown products: Not stated

Remarks:

Conclusions

Remarks: The test substance was considered readily biodegradable under the conditions of this test (Author of report).
The biodegradation of FARNIL TH-D has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch): 1A

Remarks: Reliable without restriction; guideline study.

References

Wüthrich, V. 1995. Ready biodegradability: "Manometric Respirometry Test" for FARNIL TH-D. Study number. 397708. RCC Umweltchemie AG, Itingen/BL, Germany.

Other

Last changed:	April 17, 2001
Order number for sorting:	4c
Remarks:	

3.5 BIODEGRADATION

Test Substance

Identity:	Arneel TM (CAS RN 61790-28-1; Nitriles, tallow)
Purity:	99.2%
Remarks:	

Method

Method/Guideline followed:	OECD Guidelines for Testing of Chemicals, Guideline No. 301D: Closed Bottle Test. Modifications according to ECETOC 1985 (regarding inoculum, dilution water and analyses).
Test Type:	Aerobic ready biodegradability
GLP:	Yes
Year:	1987
Contact Time:	6 weeks
Inoculum:	Activated sludge
Remarks:	The closed bottle test was carried out in dark glass 280-ml bottles with glass stoppers. Inoculum originated from activated sludge taken from a municipal wastewater treatment plant. The sludge was preconditioned in the laboratory by aerating a 1 g s.s./l suspension of the material for one week in order to reduce high residual respiration rates. The density of the inoculum in the test was 3 mg s.s./l. Because the test substance was not soluble in water, the test substance was emulsified with a nonbiodegradable emulsifier: Genapol PF40 and nonylphenol 10E05P0 in a ratio of 1:2. The amount of the emulsifier added was about 30% of the test substance weight. A number of test vessels were prepared to provide triplicate independent measurements of disssolved oxygen at each measurement period. Experimental groups included the control blank (dilution water with inoculum), test material at 2.5 mg Arneel TM/l, and emulsifier. The concentration of the test substance provided a COD of 8.06 mg/l. Measurements of dissolved oxygen were made after 2, 4 and 6 weeks of incubation. Percent biodegradation was calculated as the measured BOD divided by the COD times 100. An assessment of the toxicity of the test substance to the inoculum was made by adding test substance with sodium acetate and incubated for seven days. Measurements of dissolved oxygen were made at that time.

Results

Degradation:	After six weeks incubation, 78% biodegradation was achieved. The test substance was considered readily biodegradable.
Results:	The extent of biodegradation was 52% after two weeks, 69% after four weeks and 78% after six weeks.
Kinetic:	No information provided.
Breakdown Products:	No information provided.
Remarks:	The emulsifier was shown to be non-biodegradable. The degradation of sodium benzoate in the presence of the test substance and emulsifier indicated that the test substance was not inhibitory to the inoculum.

Conclusions

Remarks:	The ready biodegradability of the test substance in the Closed Bottle Test was adequately characterized by the study (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study (OECD).

References

Balk, F. 1987. Biodegradability of a number of nitrogen derivatives (MU-30, Akzo Chemie). Test report number D 87/16/0525B. Akzo Research, Arnhem, Holland.

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	28
Remarks:	

3.5 BIODEGRADATION

Test Substance

Identity:	Tallow Nitrile (CAS RN 61790-28-1; Nitriles, tallow)
Purity:	Purity provided as percent carbon (81.71%)
Remarks:	

Method

Method/Guideline followed:	OECD Guidelines for Testing of Chemicals, Guideline 301B
Test Type:	Aerobic ready biodegradability
GLP:	Yes
Year:	1992
Contact Time:	28 days
Inoculum:	Activated sludge
Remarks:	The ready biodegradability in the Modified Sturm Test was determined with the activated sludge for the test substance over a period of 28 days. The test substance was tested at concentrations of 5 and 10 mg/l.

Results

Degradation:	Test substance concentrations of 5 and 10 mg/l resulted in degradation of 94 and 64 %, respectively after 28 days.
Results:	The theoretical CO_2 production of the test substance at 5 and 10 mg/l was 15.0 and 29.9 mg/l, respectively. The temperature during the test ranged from 22 to 23 °C and the pH of the test water on day 27 was 7.17 to 7.19. The COD at the beginning of the test for the 5 and 10 mg/l concentrations were 15.21 and 34.70 mg/l, respectively, and < 2 mg/l for both concentrations at the end of the test.
Kinetic:	Degradation of test substance over time:

Day	5 mg/l	10 mg/l
6	30%	12%
14	57%	40%
21	60%	51%
28	94%	64%

Breakdown Products:	No information provided
Remarks:	A preliminary bacterial inhibition assay was conducted and showed that the test substance was not inhibitory to the inoculum. The biodegradation of the test substance was measured by titration. To test the inoculum and the testing conditions, an assay was run with the reference substance, natrium acetate. The reference substance was 90 % degraded after 28 days.

Conclusions

Remarks:	Degradation of the test substance at concentrations of 5 and 10 mg/l achieved 94% and 64% of the TCO_2, respectively, by day 28, indicating that the test substance was readily biodegradable under the conditions of the test. (Author of report) The ready biodegradability of the test substance in the Modified Sturm Test was adequately characterized by the study. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study (OECD)

References

Noack, M. 1992. Biodegradation of tallow nitrile in the Modified Sturm Test. Test number AST27471. Dr. U. Noack Laboratories for Applied Biology, Hildesheim, Germany.

Other Available Reports

IUCLID (update 23-Oct-95).
Hoechst: Unpublished document (Noack AST27471, 12.08.1992).

Other

Last Changed:	April 17, 2001
Order Number for Sorting:	29-37
Remarks:	

3.5 BIODEGRADATION

Test Substance

Identity:	Tallow Nitrile (CAS RN 61790-28-1; Nitriles, tallow)
Purity:	0.02 [mg KOH/g], 51.5 [g J_2/100g] and 0.05 [%] water
Remarks:	

Method

Method/Guideline followed:	OECD Guideline 301B, CO_2 Evolution Test
Test type:	Aerobic ready biodegradability
GLP:	Yes
Year:	1996
Contact time:	28 days
Inoculum:	Activated sludge
Remarks:	The ready biodegradability in the Modified Sturm Test was determined with the nonadapted activated sludge for the test substance over a period of 28 days. The test vessels contained approximately 18 x 10^2 colony forming units/ml of inoculum. The test substance was tested in a concentration of 13 mg/l in duplicates, corresponding to a carbon content of 10.6 mg C/l. The biological degradation of the test substance was followed by titrimetric analyses of the quantity of CO_2, which was produced by the respiration of bacteria. The degradation was terminated with HCl on day 28 and the last titration was made on day 29, after the soluble CO_2 was turned out over a period of 24 hours. The CO_2 production was calculated as the percentage of total CO_2 that the test substance could have theoretically produced based on carbon composition. Biodegradability was, therefore, expressed as a percentage ThCO_2 and was calculated for each titration of CO_2. In order to check the activity of the study system, sodium acetate (35 mg/l, single replicate) was used as the functional control. A negative control comprising nutrient solution and inoculum (duplicate) and a toxicity control comprising the test substance (13 mg/l) and the functional control (35 mg/l) also were tested (single replicate). The following deviations from the guideline occurred: 1) The guideline recommends the range of colony forming units between 10^6-10^8 colony forming units/ml. A bacterial density was chosen which, from experience, quickly adapted for the biodegradation of the ready biodegradable functional control. Also, the test duration of 28 days allows sufficient time for adaptation of the microorganisms to the test compounds. 2) The relation between IC and TC content of the test substance in the mineral medium was not

determined at the beginning of the test because the test substance was not fully soluble in the test medium.

Results

Degradation:	The pass level of 10% (start of the degradation phase) was reached by the test substance between the fourth and sixth days. In the 10-day window, the test substance came to a mean degradation rate of 56%. After 28 days a mean degradation rate of 72% was reached. The test substance is considered readily biodegradable under the conditions of this test.
Results:	27.8 mg/l $C0_2$ production after 28 days: $ThCo_2$ = 38.7 mg/l
Kinetic:	Degradation of test substance over time: 6 days = 16% 13 days = 56% 20 days = 63% 28 days = 72%
Breakdown products:	Not stated
Remarks:	The functional control was degraded to 72% after 13 days and, therefore, the quality criterion of "degradation > 60% after 14 days" was fulfilled. In the toxicity control the degradation came to a rate of 71% after 13 days and reached a maximum of 85% after 28 days, fulfilling the guideline criterion of "degradation > 25% after 14 days". The temperatures in the water bath during incubation times ranged from 23 to 24 °C.

Conclusions

Remarks:	The test substance could be regarded to be readily biodegradable (Author of report). The biodegradation of tallow nitrile has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Noack, M. 1996. Tallow nitrile ready biodegradability Modified Sturm Test. Study number AST49621. Dr. U. Noack-Laboratorium, Hildesheim, Germany.

Other

Last changed:	April 17, 2001
Order number for sorting:	38d
Remarks:	

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	Dodecanenitrile (CAS RN 2437-25-4)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	OECD Guideline 203 "Fish, Acute Toxicity Test"
Type:	Static
GLP:	Yes
Year:	1987
Species/Strain/Supplier:	Zebra fish (*Brachydanio rerio*)
Analytical Monitoring:	No data
Exposure Period:	96 hours
Statistical Methods:	Not stated
Remarks:	

Results

Nominal concentrations (mg/l):	Not stated
Measured concentrations (mg/l):	Not stated
Unit:	mg/l
Element Value:	96-hour LC_{50} > 1 mg/l and < 10 mg/l
Statistical Results:	Not stated
Result:	No fish died at 1 mg/l and 100 % of the fish died at 10 mg/l.
Remarks:	

Conclusions

Remarks:	The 96-hour acute toxicity of the test substance to zebra fish was adequately characterized by the report (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restriction; IUCLID summary of study conducted to guideline.

References

Hoechst. 1987. Unpublished document (87.1817). Cited in IUCLID (update 23-Oct-95).

Other Available Reports

Other

Last Changed: January 5, 2004
Order Number for Sorting: 5
Remarks:

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	Hexadecanenitrile (CAS RN 629-79-8)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Fish
Analytical monitoring:	NA
Exposure period:	96-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: octanol-water partition coefficient, Log K_{ow} = 6.0.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	96-hour LC_{50} = 0.031 mg/l
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCCCCCCCCCCCCCC
CHEM   : Hexadecanenitrile
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C16 H31 N1
MOL WT : 237.43
Log Kow: 6.00  (User entered)
Melt Pt:
Wat Sol: 0.08781 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Neutral Organics


                                                                  Predicted
ECOSAR Class              Organism        Duration  End Pt  mg/L (ppm)
========================  ==============  ========  ======  ==========
Neutral Organic SAR   : Fish            14-day    LC50       0.105 *
(Baseline Toxicity)

Neutral Organics      : Fish            96-hr     LC50       0.031
Neutral Organics      : Fish            14-day    LC50       0.105 *
Neutral Organics      : Daphnid         48-hr     LC50       0.043
Neutral Organics      : Green Algae     96-hr     EC50       0.034
Neutral Organics      : Fish            30-day    ChV        0.008
Neutral Organics      : Daphnid         16-day    EC50       0.013
Neutral Organics      : Green Algae     96-hr     ChV        0.034
Neutral Organics      : Fish  (SW)      96-hr     LC50       0.048
Neutral Organics      : Mysid Shrimp    96-hr     LC50    0.000508

                                                          mg/kg (ppm)
                                                          dry wt soil
                                                          ===========
Neutral Organics      : Earthworm       14-day    LC50      85.613 *

 Note:  * = asterick designates: Chemical may not be soluble
        enough to measure this predicted effect.
         Fish and daphnid acute toxicity log Kow cutoff: 5.0
         Green algal EC50 toxicity log Kow cutoff: 6.4
         Chronic toxicity log Kow cutoff: 8.0
         MW cutoff: 1000
```

Conclusions

The 96-hour LC_{50} for Hexadecanenitrile was calculated as 0.031 mg/l.

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 22, 2003

Order number for sorting:

Remarks:

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	Octadecanenitrile (CAS RN 638-65-3)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Fish
Analytical monitoring:	NA
Exposure period:	96-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: melting point = 41°C; boiling point = 362°C; octanol-water partition coefficient, Log K_{ow} = 6.0.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	96-hour LC_{50} = 0.034 mg/l
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCCCCCCCCCCCCCCC
CHEM   : Octadecanenitrile
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C18 H35 N1
MOL WT : 265.49
Log Kow: 6.00  (User entered)
Melt Pt: 41.00 deg C
Wat Sol: 0.2759 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Neutral Organics
```

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	0.117
Neutral Organics	: Fish	96-hr	LC50	0.034
Neutral Organics	: Fish	14-day	LC50	0.117
Neutral Organics	: Daphnid	48-hr	LC50	0.048
Neutral Organics	: Green Algae	96-hr	EC50	0.038
Neutral Organics	: Fish	30-day	ChV	0.008
Neutral Organics	: Daphnid	16-day	EC50	0.014
Neutral Organics	: Green Algae	96-hr	ChV	0.038
Neutral Organics	: Fish (SW)	96-hr	LC50	0.054
Neutral Organics	: Mysid Shrimp	96-hr	LC50	0.000568

				mg/kg (ppm) dry wt soil
Neutral Organics	: Earthworm	14-day	LC50	95.729 *

```
 Note:  * = asterick designates: Chemical may not be soluble
            enough to measure this predicted effect.
          Fish and daphnid acute toxicity log Kow cutoff: 5.0
          Green algal EC50 toxicity log Kow cutoff: 6.4
          Chronic toxicity log Kow cutoff: 8.0
          MW cutoff: 1000
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 22, 2003

Order number for sorting:

Remarks:

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	Nitriles, C16-18 (CAS RN 68002-65-3)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Fish
Analytical monitoring:	NA
Exposure period:	96-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	96-hour LC_{50} = 0.002 mg/l
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCCCCCCCCCCCCCC
CHEM   : Nitriles, C16-18
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C17 H33 N1
MOL WT : 251.46
Log Kow: 7.22  (KowWin estimate)
Melt Pt:
Wat Sol: 0.005297 mg/L  (calculated)

ECOSAR v0.99g Class(es) Found
-----------------------------
Neutral Organics


                                                          Predicted
ECOSAR Class           Organism       Duration  End Pt  mg/L (ppm)
=====================  =============  ========  ======  ==========
Neutral Organic SAR  : Fish           14-day    LC50       0.010 *
```

(Baseline Toxicity)

Neutral Organics	: Fish	96-hr	LC50	0.002	
Neutral Organics	: Fish	14-day	LC50	0.010	*
Neutral Organics	: Daphnid	48-hr	LC50	0.004	
Neutral Organics	: Green Algae	96-hr	EC50	0.003	
Neutral Organics	: Fish	30-day	ChV	0.00069	
Neutral Organics	: Daphnid	16-day	EC50	0.00179	
Neutral Organics	: Green Algae	96-hr	ChV	0.006	*
Neutral Organics	: Fish (SW)	96-hr	LC50	0.007	*
Neutral Organics	: Mysid Shrimp	96-hr	LC50	1.6e-005	

				mg/kg (ppm) dry wt soil	
Neutral Organics	: Earthworm	14-day	LC50	38.169	*

Note: * = asterick designates: Chemical may not be soluble enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: 5.0
Green algal EC50 toxicity log Kow cutoff: 6.4
Chronic toxicity log Kow cutoff: 8.0
MW cutoff: 1000

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 22, 2003
Order number for sorting:
Remarks:

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	Nitriles, C16-22 (CAS RN 68153-02-6)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Fish
Analytical monitoring:	NA
Exposure period:	96-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	96-hour LC_{50} = 0.0003 mg/l
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCCCCCCCCCCCCCCCC
CHEM   : Nitriles, C16-22
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C19 H37 N1
MOL WT : 279.51
Log Kow: 8.20  (KowWin estimate)
Melt Pt:
Wat Sol: 0.0005894 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Neutral Organics


                                                          Predicted
ECOSAR Class           Organism      Duration  End Pt   mg/L (ppm)
=====================  ============  ========  ======   ==========
Neutral Organic SAR  : Fish          14-day    LC50      0.00149 *
(Baseline Toxicity)

Neutral Organics     : Fish          96-hr     LC50     0.000308
Neutral Organics     : Fish          14-day    LC50      0.00149 *
Neutral Organics     : Daphnid       48-hr     LC50     0.000506
Neutral Organics     : Green Algae   96-hr     EC50     0.000452
Neutral Organics     : Fish          30-day    ChV      0.000108
Neutral Organics     : Daphnid       16-day    EC50     0.000391
Neutral Organics     : Green Algae   96-hr     ChV       0.00163 *
Neutral Organics     : Fish  (SW)    96-hr     LC50      0.00141 *
Neutral Organics     : Mysid Shrimp  96-hr     LC50    1.06e-006

                                                         mg/kg (ppm)
                                                         dry wt soil
                                                         ===========
Neutral Organics     : Earthworm     14-day    LC50        21.174 *

 Note:  * = asterick designates: Chemical may not be soluble
        enough to measure this predicted effect.
         Fish and daphnid acute toxicity log Kow cutoff: 5.0
         Green algal EC50 toxicity log Kow cutoff: 6.4
         Chronic toxicity log Kow cutoff: 8.0
         MW cutoff: 1000
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 23, 2003
Order number for sorting:
Remarks:

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	Nitriles, C14-18 and C16-18, unsaturated (CAS RN 68513-04-2)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Fish
Analytical monitoring:	NA
Exposure period:	96-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	96-hour LC_{50} = not toxic at solubility
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CC=CC=CCCCC=CCCCCC
CHEM   : Nitriles, C14-18 and C16-18-unsatd.
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C16 H25 N1
MOL WT : 231.38
Log Kow: 6.08  (KowWin estimate)
Melt Pt:
Wat Sol: 0.07091 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Allylic/Vinyl Nitriles


                                                                 Predicted
ECOSAR Class              Organism    Duration  End Pt   mg/L (ppm)
========================  ==========  ========  ======   ==========
Neutral Organic SAR     : Fish        14-day    LC50        0.087 *
(Baseline Toxicity)

Allylic/Vinyl Nitriles  : Fish        96-hr     LC50        0.276 *

 Note:  * = asterick designates: Chemical may not be soluble
            enough to measure this predicted effect.
         Fish and daphnid acute toxicity log Kow cutoff: 5.0
         Green algal EC50 toxicity log Kow cutoff: 6.4
         Chronic toxicity log Kow cutoff: 8.0
         MW cutoff: 1000
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 23, 2003

Order number for sorting:

Remarks:

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	Nitriles, C16 and C18 unsaturated (CAS RN 68002-64-2)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Fish
Analytical monitoring:	NA
Exposure period:	96-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	96-hour LC_{50} = 0.002 mg/l
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCCCCCCC=CCC=CCCCCC
CHEM   : Nitriles, C16 and C18-unsatd.
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C18 H31 N1
MOL WT : 261.45
Log Kow: 7.28  (KowWin estimate)
Melt Pt:
Wat Sol: 0.004784 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Neutral Organics


                                                                  Predicted
ECOSAR Class            Organism      Duration  End Pt  mg/L (ppm)
======================  ============  ========  ======  ==========
Neutral Organic SAR  : Fish          14-day    LC50       0.009 *
(Baseline Toxicity)

Neutral Organics     : Fish          96-hr     LC50       0.002
Neutral Organics     : Fish          14-day    LC50       0.009 *
Neutral Organics     : Daphnid       48-hr     LC50       0.003
Neutral Organics     : Green Algae   96-hr     EC50       0.003
Neutral Organics     : Fish          30-day    ChV     0.000636
Neutral Organics     : Daphnid       16-day    EC50     0.00168
Neutral Organics     : Green Algae   96-hr     ChV        0.006 *
Neutral Organics     : Fish  (SW)    96-hr     LC50       0.006 *
Neutral Organics     : Mysid Shrimp  96-hr     LC50     1.4e-005

                                                        mg/kg (ppm)
                                                        dry wt soil
                                                        ===========
Neutral Organics     : Earthworm     14-day    LC50       38.033 *

 Note:  * = asterick designates: Chemical may not be soluble
            enough to measure this predicted effect.
          Fish and daphnid acute toxicity log Kow cutoff: 5.0
          Green algal EC50 toxicity log Kow cutoff: 6.4
          Chronic toxicity log Kow cutoff: 8.0
          MW cutoff: 1000
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 23, 2003
Order number for sorting:
Remarks:

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	9-Octadecenenitrile, (Z)- (CAS RN 112-91-4)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Fish
Analytical monitoring:	NA
Exposure period:	96-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: melting point = -1°C and boiling point = 330°C.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	96-hour LC_{50} = 0.0013 mg/l
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCCCCCCC=CCCCCCCCC
CHEM   : 9-Octadecenenitrile, (Z)-
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C18 H33 N1
MOL WT : 263.47
Log Kow: 7.50  (KowWin estimate)
Melt Pt: -1.00 deg C
Wat Sol: 0.006155 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Neutral Organics
```

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	0.006
Neutral Organics	: Fish	96-hr	LC50	0.00132
Neutral Organics	: Fish	14-day	LC50	0.006
Neutral Organics	: Daphnid	48-hr	LC50	0.002
Neutral Organics	: Green Algae	96-hr	EC50	0.00178
Neutral Organics	: Fish	30-day	ChV	0.000413
Neutral Organics	: Daphnid	16-day	EC50	0.00118
Neutral Organics	: Green Algae	96-hr	ChV	0.004
Neutral Organics	: Fish (SW)	96-hr	LC50	0.004
Neutral Organics	: Mysid Shrimp	96-hr	LC50	7.51e-006

				mg/kg (ppm) dry wt soil
Neutral Organics	: Earthworm	14-day	LC50	32.789 *

```
 Note:  * = asterick designates: Chemical may not be soluble
            enough to measure this predicted effect.
          Fish and daphnid acute toxicity log Kow cutoff: 5.0
          Green algal EC50 toxicity log Kow cutoff: 6.4
          Chronic toxicity log Kow cutoff: 8.0
          MW cutoff: 1000
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 23, 2003

Order number for sorting:

Remarks:

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	Propionitrile, 3-(9-Octadecenylamino)- [CAS RN 26351-32-6; Propanenitrile, 3-(9-Octadecenylamino)-, (Z)-]
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Fish
Analytical monitoring:	NA
Exposure period:	96-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	96-hour LC_{50} = not toxic at solubility
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCNCCCCCCCCC=CCCCCCCCC
CHEM   : Propionitrile, 3-(9-octadecenylamino)-
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C21 H40 N2
MOL WT : 320.57
Log Kow: 7.47  (KowWin estimate)
Melt Pt:
Wat Sol: 0.003754 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Aliphatic Amines
```

ECOSAR Class		Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	:	Fish	14-day	LC50	0.007 *
Aliphatic Amines	:	Fish	96-hr	LC50	0.028 *
Aliphatic Amines	:	Daphnid	48-hr	LC50	0.004 *
Aliphatic Amines	:	Green Algae	96-hr	EC50	0.052 *
Aliphatic Amines	:	Green Algae	96-hr	ChV	0.041 *

```
 Note:  * = asterick designates: Chemical may not be soluble
            enough to measure this predicted effect.
          Fish and daphnid acute toxicity log Kow cutoff: none
          Green algal EC50 toxicity log Kow cutoff: none
          Chronic toxicity log Kow cutoff: none
          MW cutoff: none
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 26, 2003

Order number for sorting:

Remarks:

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	CESIO 43 (CAS RN 61789-53-5; Nitriles, coco)
Purity:	Purity provided as percent distribution of carbon chain lengths from C8 to C18.
Remarks:	

Method

Method/guideline followed:	OECD Guideline for Testing of Chemicals, Guideline No. 203.
Type:	Semi-static, with 24-hour renewals
GLP:	Yes
Year:	1992
Species/Strain/Supplier:	Zebra fish (*Brachydanio rerio*)/NA/Monksfield Aquatics, Cambridge
Analytical Monitoring:	Yes. Concentration verification by GC
Exposure Period:	96 hours
Statistical Methods:	Method employed computer algorithm designed by Stephan, US EPA 1982.
Remarks:	The study measured the acute toxicity of the test substance to zebra fish during a 96-hour static-renewal exposure period. Fish in holding were fed a commercial fish diet daily. Food was withheld from the fish 24 hours prior to and during testing. No mortalities occurred during the 14-day period prior to the test. Mean wet weights and mean fork lengths of a sample of fish taken from the group used in the test were 0.45 g and 3.2 cm, respectively. During the test, groups of 10 fish were exposed to the test substance in sealed vessels containing nominal concentrations of 0 (control), 0 (solvent control using acetone at 0.1 ml/l), 1, 3.2, 5.6, 10, 32 and 56 mg/l. Fish were allocated in groups of five to each vessel until each vessel contained 10 fish. Test vessels were glass aspirators with a capacity of approximately 22 liters. Before use, each vessel was silinised with a 2.0% solution of SurfaSil. Each vessel then was completely filled with test solution and sealed with a silicone bung. Test solutions were prepared by diluting concentrated aqueous dispersions in which the test substance was mixed with acetone and added directly to two liters of dilution water. The dispersion was subjected to ultrasound treatment for 30 minutes then adjusted to a final volume of

approximately 22 liters. Dilution water was dechlorinated tap water that was blended to achieve a water hardness of 200 – 250 mg/l. Fresh test solutions were prepared at each 24-hour interval. The target temperature for testing was 22 ± 1 °C. The photoperiod was 16 hours light/8 hours dark with simulated dawn and dusk periods at the beginning and end of each light phase. Fluorescent lamps provided ambient laboratory lighting. Temperature, dissolved oxygen and pH were measured daily either before or after observations for fish behavior. The total hardness in the control, low and high test levels was measured at the start and end of the test. Observations of the fish were made after 24, 48, 72 and 96 hours. Chemical analysis of test concentrations were made on two samples of test solution taken from each vessel before the addition fish and 24 hours later on two occasions (0/24 hours and 72/96 hours). Because the test material was a mixture of different fatty acid nitriles, two components having peak areas at 8.0 and 12.5 minute retention times were assayed. The exposure concentrations used for endpoint calculations were based on the more stable component (retention time of 8.0 minutes) of the mixture. The limit of the assay was 0.01 mg/l.

Results

Nominal concentrations (mg/l): 0 (control), 0 (solvent control), 1, 3.2, 5.6, 10, 32, and 56 mg/l.

Measured concentrations (mg/l):

Nominal Concentration	Time (hours)	Measured, Fresh Solutions (mg/l)	Time (hours)	Measured, Old Solutions (mg/l)
0 (control)	0	nd/nd	24	nd/nd
	72	nd/nd	96	0.03/0.03
1.0	0	0.31/0.27	24	0.48/0.50
	72	0.26/0.26	96	0.54/0.53
3.2	0	0.58/0.55	24	0.84/0.85
	72	0.41/0.44	96	0.97/0.89
5.6	0	0.98/0.87	24	1.17/1.25
	72	0.51/0.55	96	1.09/1.15
10.0	0	2.29/2.14	24	1.35/1.34
	72	2.49/2.60	96	1.75/1.67
32.0	0	5.36/5.15	24	1.84/1.96
	72	6.03/5.86	96	2.71/2.54
56.0	0	33.8/34.6	24	20.2/20.4
	72	12.5/11.5	96	4.59/4.59

Unit: mg/l

Element Value: Measured concentrations: 96-hour LC_{50} = 3.53 mg/l
Nominal concentrations: 96-hour LC_{50} = 32 mg/l

Statistical Results:	Measured concentrations: 96-hour LC_{50} = 3.53 mg/l Nominal concentrations: 96-hour LC_{50} = 32 mg/l
Result:	The highest nominal concentration at which no mortalities occurred was 5.6 mg/l and the lowest concentration at which 100% mortality occurred was 56 mg/l (mean measured values of 0.90 and 14.0 mg/l, respectively). The NOEC = 1 mg/l (nominal) and 0.38 mg/l (mean measured).
Remarks:	Treatment-related effects were observed and were progressive at concentrations of 3.2 mg/l (nominal) and above. Effects included lethargic behavior, darkened pigmentation, nervous behavior, loss of coordination, and overturned and immobile on the bottom of the vessel.

Conclusions

Remarks:	The 96-hour acute toxicity of the test substance to zebra fish was adequately characterized by the report (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction, guideline study (OECD No. 203).

References

Jenkins, W. R. 1992. CESIO 43: Acute toxicity to zebra fish. Confidential report number 92/CFY001/0180. Life Science Research Limited, Eye, Suffolk, UK.

Other Available Reports

Other

Last Changed:	January 5, 2004
Order number for sorting:	7a
Remarks:	

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	Tallow-nitriles (CAS RN 61790-28-1; Nitriles, tallow)
Purity:	Purity provided as percent distribution of carbon chain length from C_{12} to C_{20}.
Remarks:	

Method

Method/guideline followed:	OECD Guideline 203 "Fish, Acute Toxicity Test"
Type:	Static
GLP:	No
Year:	Not stated
Species/Strain/Supplier:	Zebra fish (*Brachydanio rerio*) (supplier not stated)
Analytical Monitoring:	No
Exposure Period:	96 hours
Statistical Methods:	Not stated
Remarks:	Dispersing agent = 0.1 ml Tween 80/l

Results

Nominal concentrations (mg/l):	Not stated
Measured concentrations (mg/l):	Not stated
Unit:	mg/l
Element Value:	96-hour LC_{50} > 10 < 100 mg/l
Statistical Results:	Not stated
Result:	
Remarks:	96-hour LC_0 = 10 mg/l

Conclusions

Remarks:	The 96-hour acute toxicity of the test substance to zebra fish was adequately characterized by the report (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	1D
Remarks:	Reliable without restriction; guideline study with minimal data provided.

References

Jung, A. 1988. Short report: acute toxicity to fish. Report number 88.0154. PHARMA Research Toxicology.

Other Available Reports

IUCLID (update 23-Oct-95).
Hoechst: Unpublished document (88.0154)

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	30-37
Remarks:	

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	Soy Nitrile (CAS RN 68514-67-0; Nitriles, soya)
Purity:	Approximately 10-16% C_{16} Nitrile and Approximately 78-86% C_{18} Nitrile
Remarks:	

Method

Method/guideline followed:	Guideline 92/69/EWG, Annex, Part C, "Methods for Determination of Ecotoxicity", C.1.: "Acute Toxicity to Fish", 31.07.1992 and OECD-Guideline for testing of chemicals, 203 Fish, Acute Toxicity Test, Adopted: 17.07.1992
Type:	Static
GLP:	Yes
Year:	1996
Species/Strain/Supplier:	Zebra fish (*Brachydanio rerio*) Supplier was HAMILTON-BUCHANAN/Hoechst Marion Roussel
Analytical Monitoring:	Yes; TOC-Analysis
Exposure Period:	96 hours
Statistical Methods:	Not stated
Remarks:	The study measured the acute toxicity of the test substance to zebra fish during a 96-hour exposure period. Mean body length of the fish was 2.9 cm. During the test, fish were exposed to the test substance at nominal concentrations of 0 (control), 10, 22, 50, 100, 220, 500 and 1000 mg/l. Temperature, dissolved oxygen and pH were measured daily and resulted in the following ranges:

Parameter	Test Groups	Control
pH (1)	7.7 – 8.2	7.8 – 8.0
Dissolved Oxygen (mg/l)	7.2 – 8.9	7.9 – 9.5
Temperature (C)	21.6 – 22.5	21.6 – 22.3

Observations of the fish were made after 24, 48, 72 and 96 hours. Because of the low solubility of the test material, the measured values were already slightly lower than the nominal values at the beginning of the experiment (32 – 102%), then
sank to 9 – 44%. The tested concentrations were

over the saturation point in water. The result is based on the nominal concentrations and takes into account dissolved and undissolved components of the test substance.

Results

Nominal concentrations (mg/l):	0 (control), 10, 22, 50, 100, 220, 500 and 1000 mg/l.
Measured concentrations (mg/l):	Not stated
Unit:	mg/l
Element Value:	96-hour LC_{50} = 33.2 mg/l [This was calculated as the "geometric mean" of the LC_0 (22 mg/l) and LC_{100} (50 mg/l)]
Statistical Results:	Not stated
Result:	The highest nominal concentration at which no mortalities occurred was 22 mg/l and the lowest concentration at which 100% mortality occurred was 50 mg/l.
Remarks:	In all test groups, changes in appearance and behavior were observed in comparison to the control group. Dead fish showed partial dark coloration or lightening and several had reddening of the gills and lock-jaw.

Conclusions

Remarks:	The 96-hour acute toxicity of the test substance to zebra fish was adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction, guideline study (OECD).

References

Zok, S. 1996. 96-hour acute toxicity test of soy nitrile to fish (*Brachydanio rerio*). Hoechst AG – Hoechst Marion Roussel, Preclinical
Development – Drug Safety, Frankfurt, Germany.

Other Available Reports

Other

Last Changed:	May 9, 2001
Order number for sorting:	4b
Remarks:	

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	Dodecanenitrile (CAS RN 2437-25-4)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Daphnid
Analytical monitoring:	NA
Exposure period:	48-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: octanol-water partition coefficient, Log K_{ow} = 4.9.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	48-hour LC_{50} = 0.33 mg/l
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCCCCCCCCC
CHEM   : Dodecanenitrile
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C12 H23 N1
MOL WT : 181.32
Log Kow: 4.90  (User entered)
Melt Pt:
Wat Sol: 0.8881 mg/L  (calculated)

ECOSAR v0.99g Class(es) Found
-----------------------------
```

Neutral Organics

Predicted ECOSAR Class	Organism	Duration	End Pt	mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	0.725
Neutral Organics	: Fish	96-hr	LC50	0.253
Neutral Organics	: Fish	14-day	LC50	0.725
Neutral Organics	: Daphnid	48-hr	LC50	0.331
Neutral Organics	: Green Algae	96-hr	EC50	0.244
Neutral Organics	: Fish	30-day	ChV	0.052
Neutral Organics	: Daphnid	16-day	EC50	0.060
Neutral Organics	: Green Algae	96-hr	ChV	0.131
Neutral Organics	: Fish (SW)	96-hr	LC50	0.235
Neutral Organics	: Mysid Shrimp	96-hr	LC50	0.009
				mg/kg (ppm) dry wt soil
Neutral Organics	: Earthworm	14-day	LC50	142.644 *

Note: * = asterick designates: Chemical may not be soluble enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: 5.0
Green algal EC50 toxicity log Kow cutoff: 6.4
Chronic toxicity log Kow cutoff: 8.0
MW cutoff: 1000

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 20, 2003

Order number for sorting:

Remarks:

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	Hexadecanenitrile (CAS RN 629-79-8)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Daphnid
Analytical monitoring:	NA
Exposure period:	48-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: octanol-water partition coefficient, Log K_{ow} = 4.9.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	48-hour LC_{50} = 0.043 mg/l
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCCCCCCCCCCCCCC
CHEM   : Hexadecanenitrile
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C16 H31 N1
MOL WT : 237.43
Log Kow: 6.00  (User entered)
Melt Pt:
Wat Sol: 0.08781 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Neutral Organics
```

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	0.105 *
Neutral Organics	: Fish	96-hr	LC50	0.031
Neutral Organics	: Fish	14-day	LC50	0.105 *
Neutral Organics	: Daphnid	48-hr	LC50	0.043
Neutral Organics	: Green Algae	96-hr	EC50	0.034
Neutral Organics	: Fish	30-day	ChV	0.008
Neutral Organics	: Daphnid	16-day	EC50	0.013
Neutral Organics	: Green Algae	96-hr	ChV	0.034
Neutral Organics	: Fish (SW)	96-hr	LC50	0.048
Neutral Organics	: Mysid Shrimp	96-hr	LC50	0.000508

				mg/kg (ppm) dry wt soil
Neutral Organics	: Earthworm	14-day	LC50	85.613 *

```
 Note:  * = asterisk designates: Chemical may not be soluble
        enough to measure this predicted effect.
         Fish and daphnid acute toxicity log Kow cutoff: 5.0
         Green algal EC50 toxicity log Kow cutoff: 6.4
         Chronic toxicity log Kow cutoff: 8.0
         MW cutoff: 1000
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 22, 2003

Order number for sorting:

Remarks:

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	Octadecanenitrile (CAS RN 638-65-3)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Daphnid
Analytical monitoring:	NA
Exposure period:	48-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: melting point = 41°C; boiling point = 362°C; octanol-water partition coefficient, Log K_{ow} = 6.0.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	48-hour LC_{50} = 0.048 mg/l
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCCCCCCCCCCCCCCC
CHEM   : Octadecanenitrile
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C18 H35 N1
MOL WT : 265.49
Log Kow: 6.00  (User entered)
Melt Pt: 41.00 deg C
Wat Sol: 0.2759 mg/L  (calculated)
```

ECOSAR v0.99g Class(es) Found

Neutral Organics

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	0.117
Neutral Organics	: Fish	96-hr	LC50	0.034
Neutral Organics	: Fish	14-day	LC50	0.117
Neutral Organics	: Daphnid	48-hr	LC50	0.048
Neutral Organics	: Green Algae	96-hr	EC50	0.038
Neutral Organics	: Fish	30-day	ChV	0.008
Neutral Organics	: Daphnid	16-day	EC50	0.014
Neutral Organics	: Green Algae	96-hr	ChV	0.038
Neutral Organics	: Fish (SW)	96-hr	LC50	0.054
Neutral Organics	: Mysid Shrimp	96-hr	LC50	0.000568
Neutral Organics	: Earthworm	14-day	LC50	mg/kg (ppm) dry wt soil: 95.729 *

Note: * = asterick designates: Chemical may not be soluble enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: 5.0
Green algal EC50 toxicity log Kow cutoff: 6.4
Chronic toxicity log Kow cutoff: 8.0
MW cutoff: 1000

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 22, 2003

Order number for sorting:

Remarks:

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	Nitriles, C16-18 (CAS RN 68002-65-3)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Daphnid
Analytical monitoring:	NA
Exposure period:	48-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	48-hour LC_{50} = 0.004 mg/l
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCCCCCCCCCCCCCC
CHEM   : Nitriles, C16-18
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C17 H33 N1
MOL WT : 251.46
Log Kow: 7.22  (KowWin estimate)
Melt Pt:
Wat Sol: 0.005297 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Neutral Organics


                                                                  Predicted
ECOSAR Class            Organism       Duration  End Pt  mg/L (ppm)
======================  =============  ========  ======  ==========
Neutral Organic SAR  : Fish           14-day    LC50       0.010 *
(Baseline Toxicity)

Neutral Organics     : Fish           96-hr     LC50       0.002
Neutral Organics     : Fish           14-day    LC50       0.010 *
Neutral Organics     : Daphnid        48-hr     LC50       0.004
Neutral Organics     : Green Algae    96-hr     EC50       0.003
Neutral Organics     : Fish           30-day    ChV      0.00069
Neutral Organics     : Daphnid        16-day    EC50     0.00179
Neutral Organics     : Green Algae    96-hr     ChV        0.006 *
Neutral Organics     : Fish  (SW)     96-hr     LC50       0.007 *
Neutral Organics     : Mysid Shrimp   96-hr     LC50     1.6e-005

                                                          mg/kg (ppm)
                                                          dry wt soil
                                                          ===========
Neutral Organics     : Earthworm      14-day    LC50       38.169 *

 Note:  * = asterick designates: Chemical may not be soluble
            enough to measure this predicted effect.
         Fish and daphnid acute toxicity log Kow cutoff: 5.0
         Green algal EC50 toxicity log Kow cutoff: 6.4
         Chronic toxicity log Kow cutoff: 8.0
         MW cutoff: 1000
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 22, 2003

Order number for sorting:

Remarks:

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	Nitriles, C16-22 (CAS RN 68153-02-6)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Daphnid
Analytical monitoring:	NA
Exposure period:	48-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	48-hour LC_{50} = 0.0005 mg/l
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCCCCCCCCCCCCCCCC
CHEM   : Nitriles, C16-22
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C19 H37 N1
MOL WT : 279.51
Log Kow: 8.20  (KowWin estimate)
Melt Pt:
Wat Sol: 0.0005894 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Neutral Organics


                                                                  Predicted
ECOSAR Class            Organism      Duration  End Pt  mg/L (ppm)
======================  ============  ========  ======  ==========
Neutral Organic SAR  : Fish          14-day    LC50     0.00149 *
(Baseline Toxicity)

Neutral Organics     : Fish          96-hr     LC50    0.000308
Neutral Organics     : Fish          14-day    LC50     0.00149 *
Neutral Organics     : Daphnid       48-hr     LC50    0.000506
Neutral Organics     : Green Algae   96-hr     EC50    0.000452
Neutral Organics     : Fish          30-day    ChV     0.000108
Neutral Organics     : Daphnid       16-day    EC50    0.000391
Neutral Organics     : Green Algae   96-hr     ChV      0.00163 *
Neutral Organics     : Fish  (SW)    96-hr     LC50     0.00141 *
Neutral Organics     : Mysid Shrimp  96-hr     LC50   1.06e-006

                                                       mg/kg (ppm)
                                                        dry wt soil
                                                       ===========
Neutral Organics     : Earthworm     14-day    LC50       21.174 *

 Note:  * = asterick designates: Chemical may not be soluble
        enough to measure this predicted effect.
         Fish and daphnid acute toxicity log Kow cutoff: 5.0
         Green algal EC50 toxicity log Kow cutoff: 6.4
         Chronic toxicity log Kow cutoff: 8.0
         MW cutoff: 1000
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 23, 2003

Order number for sorting:

Remarks:

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	Nitriles, C14-18 and C16-18, unsaturated (CAS RN 68513-04-2)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Daphnid
Analytical monitoring:	NA
Exposure period:	48-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	48-hour LC_{50} = not calculable
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CC=CC=CCCCC=CCCCCC
CHEM   : Nitriles, C14-18 and C16-18-unsatd.
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C16 H25 N1
MOL WT : 231.38
Log Kow: 6.08  (KowWin estimate)
Melt Pt:
Wat Sol: 0.07091 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Allylic/Vinyl Nitriles


                                                                  Predicted
ECOSAR Class              Organism    Duration  End Pt   mg/L (ppm)
========================  ==========  ========  ======   ==========
Neutral Organic SAR     : Fish        14-day    LC50        0.087 *
(Baseline Toxicity)

Allylic/Vinyl Nitriles  : Fish        96-hr     LC50        0.276 *

 Note:  * = asterick designates: Chemical may not be soluble
            enough to measure this predicted effect.
         Fish and daphnid acute toxicity log Kow cutoff: 5.0
         Green algal EC50 toxicity log Kow cutoff: 6.4
         Chronic toxicity log Kow cutoff: 8.0
         MW cutoff: 1000
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 23, 2003

Order number for sorting:

Remarks:

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	Nitriles, C16 and C18 unsaturated (CAS RN 68002-64-2)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Daphnid
Analytical monitoring:	NA
Exposure period:	48-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	48-hour LC_{50} = 0.003 mg/l
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCCCCCCC=CCC=CCCCCC
CHEM   : Nitriles, C16 and C18-unsatd.
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C18 H31 N1
MOL WT : 261.45
Log Kow: 7.28  (KowWin estimate)
Melt Pt:
Wat Sol: 0.004784 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Neutral Organics


                                                                  Predicted
ECOSAR Class            Organism      Duration  End Pt  mg/L (ppm)
======================  ============  ========  ======  ==========
Neutral Organic SAR  : Fish          14-day    LC50       0.009 *
(Baseline Toxicity)

Neutral Organics     : Fish          96-hr     LC50       0.002
Neutral Organics     : Fish          14-day    LC50       0.009 *
Neutral Organics     : Daphnid       48-hr     LC50       0.003
Neutral Organics     : Green Algae   96-hr     EC50       0.003
Neutral Organics     : Fish          30-day    ChV     0.000636
Neutral Organics     : Daphnid       16-day    EC50     0.00168
Neutral Organics     : Green Algae   96-hr     ChV        0.006 *
Neutral Organics     : Fish  (SW)    96-hr     LC50       0.006 *
Neutral Organics     : Mysid Shrimp  96-hr     LC50     1.4e-005

                                                        mg/kg (ppm)
                                                        dry wt soil
                                                        ===========
Neutral Organics     : Earthworm     14-day    LC50       38.033 *

 Note:  * = asterick designates: Chemical may not be soluble
            enough to measure this predicted effect.
          Fish and daphnid acute toxicity log Kow cutoff: 5.0
          Green algal EC50 toxicity log Kow cutoff: 6.4
          Chronic toxicity log Kow cutoff: 8.0
          MW cutoff: 1000
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 23, 2003

Order number for sorting:

Remarks:

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	9-Octadecenenitrile, (Z)- (CAS RN 112-91-4)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Daphnid
Analytical monitoring:	NA
Exposure period:	48-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: melting point = -1°C and boiling point = 330°C.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	48-hour LC_{50} = 0.002 mg/l
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCCCCCCC=CCCCCCCCC
CHEM   : 9-Octadecenenitrile, (Z)-
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C18 H33 N1
MOL WT : 263.47
Log Kow: 7.50  (KowWin estimate)
Melt Pt: -1.00 deg C
Wat Sol: 0.006155 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Neutral Organics
```

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	0.006
Neutral Organics	: Fish	96-hr	LC50	0.00132
Neutral Organics	: Fish	14-day	LC50	0.006
Neutral Organics	: Daphnid	48-hr	LC50	0.002
Neutral Organics	: Green Algae	96-hr	EC50	0.00178
Neutral Organics	: Fish	30-day	ChV	0.000413
Neutral Organics	: Daphnid	16-day	EC50	0.00118
Neutral Organics	: Green Algae	96-hr	ChV	0.004
Neutral Organics	: Fish (SW)	96-hr	LC50	0.004
Neutral Organics	: Mysid Shrimp	96-hr	LC50	7.51e-006

				mg/kg (ppm) dry wt soil
Neutral Organics	: Earthworm	14-day	LC50	32.789 *

```
 Note:  * = asterick designates: Chemical may not be soluble
            enough to measure this predicted effect.
          Fish and daphnid acute toxicity log Kow cutoff: 5.0
          Green algal EC50 toxicity log Kow cutoff: 6.4
          Chronic toxicity log Kow cutoff: 8.0
          MW cutoff: 1000
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 23, 2003

Order number for sorting:

Remarks:

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	Propionitrile, 3-(9-Octadecenylamino)- [CAS RN 26351-32-6; Propanenitrile, 3-(9-Octadecenylamino)-, (Z)-]
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Daphnid
Analytical monitoring:	NA
Exposure period:	48-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	48-hour LC_{50} = not toxic at solubility
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCNCCCCCCCCC=CCCCCCCCC
CHEM   : Propionitrile, 3-(9-octadecenylamino)-
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C21 H40 N2
MOL WT : 320.57
Log Kow: 7.47  (KowWin estimate)
Melt Pt:
Wat Sol: 0.003754 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Aliphatic Amines
```

ECOSAR Class		Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	:	Fish	14-day	LC50	0.007 *
Aliphatic Amines	:	Fish	96-hr	LC50	0.028 *
Aliphatic Amines	:	Daphnid	48-hr	LC50	0.004 *
Aliphatic Amines	:	Green Algae	96-hr	EC50	0.052 *
Aliphatic Amines	:	Green Algae	96-hr	ChV	0.041 *

```
 Note:  * = asterick designates: Chemical may not be soluble
            enough to measure this predicted effect.
          Fish and daphnid acute toxicity log Kow cutoff: none
          Green algal EC50 toxicity log Kow cutoff: none
          Chronic toxicity log Kow cutoff: none
          MW cutoff: none
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 26, 2003

Order number for sorting:

Remarks:

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	CESIO 41 (CAS RN 61789-53-5; Nitriles, coco)
Purity:	Purity given as percent distribution of carbon chains C8 to C18.
Remarks:	

Method

Method/guideline followed:	OECD Guidelines for Testing of Chemicals, Guideline 202, Part 1, *Daphnia* sp., Acute Immobilization Test and Reproduction Test.
Type:	Static acute
GLP:	Yes
Year:	1992
Species/Strain/Supplier:	*Daphnia magna*/University of Sheffield/Laboratory culture
Analytical Monitoring:	Yes. Concentration verification by GC
Exposure Period:	48 hours
Statistical Methods:	Method employed computer algorithm designed by Stephan, US EPA 1982.
Remarks:	The experiment measured the survival of *Daphnia magna* over a 48-hour exposure to the test substance. Daphnids were cultured and tested in dechlorinated tap water that had been adjusted to a hardness of 200-250 mg/l as $CaCO_3$. Daphnids were exposed in groups of 20 to test substance concentrations of 0 (control), 0 (solvent control – acetone at 0.1 ml/l), 6.25, 12.5, 25, 50, and 100 µg/l. Test solutions were prepared by mixing test substance with acetone (1 mg/ml) and adding water to make 100 mg/l. This stock solution was treated to ultrasound for 30 minutes then diluted to a nominal concentration of 100 µg/l and treated to ultrasound for an additional 30 minutes. Dilutions of the 100 µg/l were done to create the lower test concentrations. Each treatment was replicated four times with each replicate test vessels holding five daphnids. Test vessels were crystallizing dishes of approximately 150-ml capacity and were covered with a watch glass during the test. At test initiation daphnids between six and 24 hours of age were collected from isolated adults and randomly distributed to the test vessels. The test vessels were placed on a laboratory bench under ambient laboratory conditions. A 16-hour light/8-hour dark photoperiod was provided using fluorescent lights. Dawn and dusk periods were simulated by a period of subdued lighting at the beginning and end of the light phase.

Dissolved oxygen (DO), water pH, and temperature were measured at the start and end of the test. The target test temperature was 20 ± 2 °C. During the test, the temperature ranged from 18.1 to 20.2 °C, pH ranged from 7.4 to 8.2, dissolved oxygen ranged from 90 to 98% air saturation, total hardness ranged from 210 to 216 mg/l as $CaCO_3$, and alkalinity ranged from 128 to 133 mg/l as $CaCO_3$.The numbers of mobile, immobile and floating daphnids were recorded after 24 and 48 hours. Notes regarding the appearance of the test solutions were made at the start and end of the test. EC_{50} concentrations were based on nominal and
0-hour measured concentrations.

Results

Nominal concentrations (mg/l):	0 (control), 0 (solvent control – acetone at 0.1 ml/l), 6.25, 12.5, 25, 50, and 100 µg/l. Concentrations were based on total product.
Measured concentrations (mg/l):	Duplicate measurements of one control, and 6.25, 12.5, 25, 50 and 100 µg/l test levels at 0 and 48 hours: 0-Hours: nd/nd (not detected), 4.6/3.3, 7.3/7.5, 16/25, 33/33, and 80/62 µg/l 48-Hours: nd/nd, nd/nd, nd/nd, nd/nd, 3/3, and 24/20 µg/l.
Unit:	µg/l
EC_{50} (48 hour):	Based on 0-Hour analytical**:** 33 µg/l (95% C.L. = 27 and 41 µg/l) Based on Nominal: 46 µg/l (95% C.L. = 37 and 58 µg/l)
LC_{50} (48 hour):	Not stated.
NOEC (48 hour):	12.5 µg/l (nominal) 7.4 µg/l (initial measured)
Result:	Additional results included the 24-hour EC_{50} = 40 µg/l (based on 0-hour analytical) and 58 µg/l (nominal). The highest nominal concentration at which no immobilization occurred was 12.5 µg/l and the highest nominal concentration of 100 µg/l resulted in 95% immobilization.
Remarks:	The limit of the analytical assay was 10 µg/l. Therefore, any measured values obtained in the 6.25 µg/l treatment were estimated. The analytical results show that although satisfactory dispersions of the test material were prepared at the start (initial measured values were between 59 and 82% nominal), they could not be maintained. This was attributed to physical instability of the dispersion. All exposure concentrations appeared clear and colorless.

Conclusions

Remarks:	The acute toxicity of the test substance to *Daphnia magna* was adequately characterized by the study (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restrictions, guideline study (OECD).

References

Jenkins, W. R. 1992. CESIO 41: Acute toxicity to *Daphnia magna*. Final report number 92/CFY002/0181. Life Science Research Limited, Eye, Suffolk, UK.

Other Available Reports

Other

Last Changed:	January 5, 2004
Order number for sorting:	8a
Remarks:	

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	Coco Nitrile (CAS RN 61789-53-5; Nitriles, Coco)
Purity:	47 – 57% C_{12}-CN (other components: C_8-CN, C_{10}-CN, C_{14}-CN, C_{16}-CN, C_{18}-CN)
Remarks:	

Method

Method/guideline followed:	92/69/EEC;Annex V; Methods for the Determination of Ecotoxicity C.2 Acute Toxicity for *Daphnia* and OECD-Guideline for testing of chemicals, Section 1 – Effects on Biotic Systems Test Guideline 202 *Daphnia sp*., 14-day Reproduction Test (including an Acute Immobilisation Test); Adopted: 04. April 1984
Type:	Not stated
GLP:	Yes
Year:	1994
Species/Strain/Supplier:	*Daphnia magna*/Hoechst AG Department of Toxicology
Analytical Monitoring:	No
Exposure Period:	48 hours
Statistical Methods:	Not stated
Remarks:	

Results

Nominal concentrations (mg/l):	0 (control), 0 (control solution with ethanol), 0.01, 0.018, 0.035, 0.056, 0.1, 0.18, 0.32, 0.56 and 1.0 mg/l
Measured concentrations (mg/l):	Not stated
Unit:	mg/l
EC_{50} (24 hour):	> 1 mg/l
EC_{50} (48 hour):	0.091 mg/l (0.076 – 0.109 confidence interval)
NOEC:	EC_0 = 0.032
Result:	
Remarks:	The following parameters were measured throughout the 48-hour exposure period and the results are listed below: pH = 8.3 to 8.6; oxygen concentration = 6.9 to 8.7 mg/l temperature = 20.8 to 21.3 °C.

Conclusions

Remarks:	The 48-hour acute toxicity of the test substance to Daphnia magna was adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study (OECD).

References

Zok and Jung. 1994. 48-hour acute toxicity to *Daphnia magna* of coco nitrile. Report number 94.0307. Pharma Entwicklung Zentrale Toxikologie, Hoechst Aktiengesellschaft, Frankfurt, Germany.

Other Available Reports

Other

Last Changed:	April 17, 2001
Order number for sorting:	20a
Remarks*:*	

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	FARNIL TH-D (CAS RN 61790-29-2; Nitriles, tallow, hydrogenated)
Purity:	100% technical grade
Remarks:	

Method

Method/Guideline followed:	OECD Guideline 202, Part 1: "*Daphnia* sp., 24 h EC_{50} Acute Immobilization Test" and Directive 92/69 EEC, C.2 of July 31, 1992 (EEC Publication No. L383 A, December 1992): "Acute Toxicity for Daphnia".
Test type:	Static
GLP:	Yes
Year:	1995
Analytical procedures:	No
Species/Strain:	*Daphnia magna*
Test details:	Static
Statistical methods:	48-hour EC_{50} by the Logit model; 48-hour EC_0 and EC_{100} by linear regression
Remarks:	The experiment measured the survival (in terms of mobility) of *Daphnia magna* over a 48-hour exposure period to the test and control substances. Daphnids were cultured at the laboratory under standardized conditions. Daphnids less than 24-hours old were exposed to the following six concentrations of the test substance: 0.070, 0.124, 0.251, 0.466, 4.9 and 9.8 mg/l. In preparation of the test concentrations, all test flasks were stirred for about 8 hours and afterwards heated to about 30 °C in an incubator for 16 hours (while being stirred continuously). The test substance melted and the solutions appeared homogeneous. After the 24-hour stirring period, the solutions were allowed to cool to room temperature and the test substance solidified. After 10 minutes sonication the test solutions of the 0.070, 0.124 and 0.251 mg/l concentrations appeared to be clear whereas the 0.466 mg/l concentration appeared to be clear but substance adhered to glass and weighing dish (aluminum). The two highest test concentrations, 4.9 and 9.8 mg/l, appeared to be slightly turbid and undissolved particles were observed. Each solution was filtered through an untreated folded filter paper and the filtrates were used in the test. Filtered and unfiltered test medium media was were used as the controls. The reference compound was

potassium dichromate. Treatments were replicated twice with 10 daphnids per replicate (20 daphnids per experimental group). Test vessels were 1- or 5-liter flasks. The pH of the untreated test medium was 8.2 at the beginning of the 48-hour exposure period. The pH ranged from 8.1 to 8.2 for all test substance concentrations and for the controls at the beginning and at the end of the test. The oxygen concentration of the untreated test medium was adjusted to 8.2 mg O_2/l at the beginning of the 48-hour exposure period. The oxygen concentration ranged from 7.3 to 8.1 mg O_2/l for all test substance concentrations and for the controls at the beginning and 8.4 to 8.6 mg O_2/l at the end of the test. Room temperature was recorded continuously and ranged from 18.0 to 20.5°C. The mobility of the daphnids after 24 and 48 hours was determined according to the guidelines.

Results

Nominal concentrations (mg/l):	0 (control), 0.070, 0.124, 0.251, 0.466, 4.9 and 9.8 mg/l
Measured concentrations (mg/l):	Not measured
Unit:	mg/l
EC_{50} (24-hour):	> 9.8 mg/l (95% confidence limits: 0.138 – 0.324 mg/l) (experimentally determined)
EC_{50} (48-hour):	> 0.216 mg/l (95% confidence limits: 0.138 – 0.324 mg/l)
Statistical results:	Described above
Remarks:	After 24 hours of exposure, no immobility was observed at the lowest two test concentrations of 0.070 and 0.124 mg/l. The immobility in all other test concentrations was in the range of 20 to 50%. After 48 hours of exposure, immobility rates, on average, of 10% were observed at the lowest two test concentrations of 0.070 and 0.124 mg/l. The concentrations 0.251 and 0.466 mg/l caused, on average, immobility rates of 75 and 95%, respectively. The two highest concentrations, 4.9 and 9.8 mg/l caused 100% immobility. No immobilization was observed in the control groups over the 48-hour exposure period.

Conclusions

Remarks:	The 48-hour acute toxicity FARNIL TH-D to *Daphnia magna* has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Nitriles Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Wüthrich, V. 1995. 48-hour acute toxicity of FARNIL TH-D to *Daphnia magna* (OECD – immobilization test). Study number 397697. RCC Umweltchemie AG, Itingen/BL, Germany.

Other

Last changed:	April 17, 2001
Order number for sorting:	4e
Remarks:	

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	CESIO 42 (CAS RN 61790-28-1; Nitriles, tallow)
Purity:	Purity provided as percentages of carbon chain lengths C14, C16 and C18.
Remarks:	

Method

Method/guideline followed:	OECD Guidelines for Testing of Chemicals, Guideline 202, Part I. *Daphnia sp*., Acute Immobilization Test and Reproduction Test. Adopted April 1984.
Type:	Static
GLP:	Yes
Year:	1992
Species/Strain/Supplier:	*Daphnia magna*/University of Sheffield/Univ. Sheffield
Analytical Monitoring:	Yes. Exposure levels were monitored by GC analysis.
Exposure Period:	48 Hours
Statistical Methods:	Method employed computer algorithm designed by Stephan, US EPA 1982.
Remarks:	The experiment measured the survival of *Daphnia magna* over a 48-hour exposure to the test substance. Daphnids were cultured and tested in dechlorinated tap water that had been adjusted to a hardness of 200 - 250 mg/l as $CaCO_3$. Daphnids were exposed in groups of 20 to test substance concentrations of 0 (control), 0 (solvent control – acetone at 0.1 ml/l), 3.13, 6.25, 12.5, 25, 50, and 100 µg/l. Test solutions were prepared by mixing test substance with acetone (1 mg/ml) and adding water to make 100 mg/l. This stock solution was treated to ultrasound for 30 minutes then diluted to a nominal concentration of 100 µg/l and treated to ultrasound for an additional 30 minutes. Dilutions of the 100 µg/l were done to create the lower test concentrations. Each treatment was replicated four times with each replicate test vessels holding five daphnids. Test vessels were crystallizing dishes of approximately 150-ml capacity and were covered with a watch glass during the test. At test initiation daphnids between six and 24 hours of age were collected from isolated adults and randomly distributed to the test vessels. The test vessels were placed on a laboratory bench under ambient laboratory conditions. A 16-hour light/8-hour dark photoperiod was provided using fluorescent lights. Dawn and dusk periods were simulated by a period of subdued lighting at the beginning and end of the light phase. Dissolved oxygen

(DO), water pH, and temperature were measured at the start and end of the test. The target test temperature was 20 ± 2 °C. During testing, the temperature ranged from 20.5 to 21.1 °C, pH ranged from 7.6 to 8.4, dissolved oxygen ranged from 90 to 96% air saturation, total hardness ranged from 218 to 236 mg/l as $CaCO_3$, and alkalinity ranged from 118 to 133 µg/l. The numbers of mobile, immobile and floating daphnids were recorded after 24 and 48 hours. Notes regarding the appearance of the test solutions were made at the start and end of the test. EC_{50} concentrations were based on nominal and 0-hour measured concentrations.

Results

Nominal concentrations (mg/l):	0 (control), 0 (acetone solvent control), 3.13, 6.25, 12.5, 25, 50 and 100 µg/l. Concentrations were based on total product.
Measured concentrations (mg/l):	Duplicate measurements of one control, and 3.13, 6.25, 12.5, 25, 50 and 100 µg/l test levels at 0 and 48 hours: 0-Hours: nd/nd (not detected), nd/nd, 8.4/8.4, 13.8/17.3, 24.9/24.3, 54.1/58.0, and 98.6/82.9 µg/l. 48-Hours: nd/nd, 8.7/nd, nd/nd, nd/nd, nd/nd, 8.2/40, and 15.9/19.6 µg/l.
Unit:	µg/l
EC_{50} (48 hour):	Based on 0-Hour analytical: 5.0 µg/l Based on Nominal: 11.9 µg/l
LC_{50} (48 hour):	Not stated
NOEC (48 hour):	6.25 µg/l (nominal concentration)
Result:	Additional results included the 24-hour EC_{50} = 58.8 µg/l (based on 0-hour analytical) and 53.5 µg/l (nominal). The highest nominal concentration at which no immobilization occurred was 6.25 µg/l and the lowest nominal concentration at which 100% immobilization occurred was 100 µg/l.
Remarks:	The limit of the analytical assay was 10 µg/l. Therefore, any measured values obtained in the 3.13 and 6.25 µg/l treatments were estimated. The analytical results show that although satisfactory dispersions of the test material were prepared at the start, they could not be maintained, which was attributed to physical instability of the dispersion.

Conclusions

Remarks:	The 48-hour acute toxicity of the test substance to *Daphnia magna* was adequately characterized by the report (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study (OECD)

References

Jenkins, W. R. 1992. CESIO 42: Acute toxicity to *Daphnia magna*. Confidential report number 92/CFY005/0228. Life Science Research Limited, Eye, Suffolk, UK.

Other Available Reports

Other

Last Changed:	January 5, 2004
Order number for sorting:	31
Remarks:	

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	Tallow-Nitrile (CAS RN 61790-28-1; Nitriles, tallow)
Purity:	100%
Remarks:	

Method

Method/guideline followed:	EWG-Guideline 84/449 L 251/155, Official document of the European Community
Type:	Not stated
GLP:	Yes
Year:	1992
Species/Strain/Supplier:	*Daphnia magna* STRAUS/Dr. U. Novack-Laboratory for Applied Biology
Analytical Monitoring:	No
Exposure Period:	48 hours
Statistical Methods:	Method employed Water Examination Bd. II (1982); VEB Gustav Fischer Publishers
Remarks:	The experiment measured the survival of *Daphnia magna* over a 48-hour exposure to the test substance. Daphnids were cultured and tested in regional tap water that had been filtered over activated charcoal. A 24-hour positive control was conducted using a 10-mg/l stock solution of the reference substance, Kaliumdichromate p. a., at concentrations of 0.32, 0.58, 1.0, 1.8 and 3.2 mg/l. The range of validity for the reference substance is $0.9 < EC_{50} < 1.9$ mg/l, or 10% immobilization of the Daphnids at the end of 24 hours. Test substance concentrations were 0 (control), 0.1, 0.18, 0.32, 0.58, 1.0, 1.8, 3.2, 5.8, 10.0 and 18 mg/l. In addition, the carrier substance, Tween 80, was tested at the highest concentration of 18 mg/l, as a control measure. Stock test solutions were prepared by mixing 100 ml test substance with 100 ml Tween 80. This stock solution was treated to ultrasound for 30 minutes and diluted with dilution water to achieve test concentrations. Daphnids were exposed to each test substance concentration in groups of 20 individuals, with each treatment being replicated four times and each replicate test vessel holding five daphnids. Test vessels were 50-ml beakers. At test initiation daphnids between two- and 24-hours of age were collected from isolated adults and randomly distributed to the test vessels. The test vessels were placed in a climate cabinet at 21 $\pm$ 1 C. A 10-hour light/14-hour dark photoperiod was provided. Dissolved oxygen (DO), water pH, and temperature were measured at

	the start and at the end of the test. The target test temperature was 21 ± 1 C. During testing, the temperature ranged from 21.4 to 21.6 °C, pH ranged from 8.19 to 8.50, dissolved oxygen ranged from7.9 to 8.1 %. The percent mobility was recorded at 24 and 48 hours.

Results

Nominal concentrations (mg/l):	0 (control), 18.0 (carrier control), 0.1, 0.18, 0.32, 0.58, 1.0, 1.8, 3.2, 5.8, 10.0 and 18 mg/l. Concentrations were based on total product.
Measured concentrations (mg/l)*:*	Not stated
Unit:	mg/l
EC_{50} (24 hour)	Based on Nominal: 2.5 mg/l
EC_{50} (48 hour):	Based on Nominal: 0.26 mg/l with a confidence interval of 0.17 to 0.4 mg/l
NOEC (48 hour):	Based on Nominal: $EC_0 < 0.1$ mg/l
Result:	The highest nominal concentration at which no immobilization occurred was < 0.1 mg/l and the lowest nominal concentration at which 100% immobilization occurred was 1.0 mg/l.
Remarks:	

Conclusions

Remarks:	The 48-hour acute toxicity of the test substance to *Daphnia magna* was adequately characterized by the report. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study (OECD).

References

Noack, M. 1984. Acute toxicity (48-hour) of tallow nitrile to *Daphnia magna* STRAUS. Test number DAT27471. Dr. U. Noack-Laboratory for Applied Biology. Hildesheim, Germany.

Other Available Reports IUCLID (update 23-Oct-95).
Hoechst: Unpublished document (Noack DAT27471, 26.06.1992).

Other

Last Changed:	April 17, 2001
Order number for sorting:	32-37
Remarks:	

4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)

Test Substance

Identity:	Dodecanenitrile (CAS RN 2437-25-4)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Green Algae
Analytical monitoring:	NA
Exposure period:	96-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: octanol-water partition coefficient, Log K_{ow} = 4.9.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	96-hour EC_{50} = 0.24 mg/l
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCCCCCCCCC
CHEM   : Dodecanenitrile
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C12 H23 N1
MOL WT : 181.32
Log Kow: 4.90  (User entered)
Melt Pt:
Wat Sol: 0.8881 mg/L  (calculated)

ECOSAR v0.99g Class(es) Found
-----------------------------
```

Neutral Organics

Predicted ECOSAR Class	Organism	Duration	End Pt	mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	0.725
Neutral Organics	: Fish	96-hr	LC50	0.253
Neutral Organics	: Fish	14-day	LC50	0.725
Neutral Organics	: Daphnid	48-hr	LC50	0.331
Neutral Organics	: Green Algae	96-hr	EC50	0.244
Neutral Organics	: Fish	30-day	ChV	0.052
Neutral Organics	: Daphnid	16-day	EC50	0.060
Neutral Organics	: Green Algae	96-hr	ChV	0.131
Neutral Organics	: Fish (SW)	96-hr	LC50	0.235
Neutral Organics	: Mysid Shrimp	96-hr	LC50	0.009

				mg/kg (ppm) dry wt soil
Neutral Organics	: Earthworm	14-day	LC50	142.644 *

Note: * = asterick designates: Chemical may not be soluble enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: 5.0
Green algal EC50 toxicity log Kow cutoff: 6.4
Chronic toxicity log Kow cutoff: 8.0
MW cutoff: 1000

Conclusions The 96-hour EC_{50} for Dodecanenitrile was calculated as 0.24 mg/l.

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 20, 2003

Order number for sorting:

Remarks:

4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)

Test Substance

Identity:	Hexadecanenitrile (CAS RN 629-79-8)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Green Algae
Analytical monitoring:	NA
Exposure period:	96-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: octanol-water partition coefficient, Log K_{ow} = 6.0.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	96-hour EC_{50} = 0.034 mg/l
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCCCCCCCCCCCCCC
CHEM   : Hexadecanenitrile
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C16 H31 N1
MOL WT : 237.43
Log Kow: 6.00  (User entered)
Melt Pt:
Wat Sol: 0.08781 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Neutral Organics
```

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	0.105 *
Neutral Organics	: Fish	96-hr	LC50	0.031
Neutral Organics	: Fish	14-day	LC50	0.105 *
Neutral Organics	: Daphnid	48-hr	LC50	0.043
Neutral Organics	: Green Algae	96-hr	EC50	0.034
Neutral Organics	: Fish	30-day	ChV	0.008
Neutral Organics	: Daphnid	16-day	EC50	0.013
Neutral Organics	: Green Algae	96-hr	ChV	0.034
Neutral Organics	: Fish (SW)	96-hr	LC50	0.048
Neutral Organics	: Mysid Shrimp	96-hr	LC50	0.000508

				mg/kg (ppm) dry wt soil
Neutral Organics	: Earthworm	14-day	LC50	85.613 *

```
 Note:  * = asterick designates: Chemical may not be soluble
        enough to measure this predicted effect.
         Fish and daphnid acute toxicity log Kow cutoff: 5.0
         Green algal EC50 toxicity log Kow cutoff: 6.4
         Chronic toxicity log Kow cutoff: 8.0
         MW cutoff: 1000
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 22, 2003

Order number for sorting:

Remarks:

4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)

Test Substance

Identity:	Octadecanenitrile (CAS RN 638-65-3)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Green Algae
Analytical monitoring:	NA
Exposure period:	96-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: melting point = 41°C; boiling point = 362°C; octanol-water partition coefficient, Log K_{ow} = 6.0.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	96-hour EC_{50} = 0.038 mg/l
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCCCCCCCCCCCCCCC
CHEM   : Octadecanenitrile
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C18 H35 N1
MOL WT : 265.49
Log Kow: 6.00  (User entered)
Melt Pt: 41.00 deg C
Wat Sol: 0.2759 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Neutral Organics
```

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	0.117
Neutral Organics	: Fish	96-hr	LC50	0.034
Neutral Organics	: Fish	14-day	LC50	0.117
Neutral Organics	: Daphnid	48-hr	LC50	0.048
Neutral Organics	: Green Algae	96-hr	EC50	0.038
Neutral Organics	: Fish	30-day	ChV	0.008
Neutral Organics	: Daphnid	16-day	EC50	0.014
Neutral Organics	: Green Algae	96-hr	ChV	0.038
Neutral Organics	: Fish (SW)	96-hr	LC50	0.054
Neutral Organics	: Mysid Shrimp	96-hr	LC50	0.000568

				mg/kg (ppm) dry wt soil
Neutral Organics	: Earthworm	14-day	LC50	95.729 *

```
 Note:  * = asterick designates: Chemical may not be soluble
            enough to measure this predicted effect.
          Fish and daphnid acute toxicity log Kow cutoff: 5.0
          Green algal EC50 toxicity log Kow cutoff: 6.4
          Chronic toxicity log Kow cutoff: 8.0
          MW cutoff: 1000
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 22, 2003

Order number for sorting:

Remarks:

4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)

Test Substance

Identity:	Nitriles, C16-18 (CAS RN 68002-65-3)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Green Algae
Analytical monitoring:	NA
Exposure period:	96-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	96-hour EC_{50} = 0.003 mg/l
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCCCCCCCCCCCCCC
CHEM   : Nitriles, C16-18
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C17 H33 N1
MOL WT : 251.46
Log Kow: 7.22  (KowWin estimate)
Melt Pt:
Wat Sol: 0.005297 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Neutral Organics


                                                                  Predicted
ECOSAR Class            Organism       Duration  End Pt  mg/L (ppm)
======================  =============  ========  ======  ==========
Neutral Organic SAR  : Fish           14-day    LC50       0.010 *
(Baseline Toxicity)

Neutral Organics     : Fish           96-hr     LC50       0.002
Neutral Organics     : Fish           14-day    LC50       0.010 *
Neutral Organics     : Daphnid        48-hr     LC50       0.004
Neutral Organics     : Green Algae    96-hr     EC50       0.003
Neutral Organics     : Fish           30-day    ChV      0.00069
Neutral Organics     : Daphnid        16-day    EC50     0.00179
Neutral Organics     : Green Algae    96-hr     ChV        0.006 *
Neutral Organics     : Fish  (SW)     96-hr     LC50       0.007 *
Neutral Organics     : Mysid Shrimp   96-hr     LC50     1.6e-005

                                                          mg/kg (ppm)
                                                          dry wt soil
                                                          ===========
Neutral Organics     : Earthworm      14-day    LC50       38.169 *

 Note:  * = asterick designates: Chemical may not be soluble
            enough to measure this predicted effect.
         Fish and daphnid acute toxicity log Kow cutoff: 5.0
         Green algal EC50 toxicity log Kow cutoff: 6.4
         Chronic toxicity log Kow cutoff: 8.0
         MW cutoff: 1000
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 22, 2003

Order number for sorting:

Remarks:

4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)

Test Substance

Identity:	Nitriles, C16-22 (CAS RN 68153-02-6)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Green Algae
Analytical monitoring:	NA
Exposure period:	96-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	96-hour EC_{50} = 0.0004 mg/l
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCCCCCCCCCCCCCCCC
CHEM   : Nitriles, C16-22
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C19 H37 N1
MOL WT : 279.51
Log Kow: 8.20  (KowWin estimate)
Melt Pt:
Wat Sol: 0.0005894 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Neutral Organics


                                                                  Predicted
ECOSAR Class            Organism      Duration  End Pt  mg/L (ppm)
======================  ============  ========  ======  ==========
Neutral Organic SAR  : Fish          14-day    LC50     0.00149 *
(Baseline Toxicity)

Neutral Organics     : Fish          96-hr     LC50    0.000308
Neutral Organics     : Fish          14-day    LC50     0.00149 *
Neutral Organics     : Daphnid       48-hr     LC50    0.000506
Neutral Organics     : Green Algae   96-hr     EC50    0.000452
Neutral Organics     : Fish          30-day    ChV     0.000108
Neutral Organics     : Daphnid       16-day    EC50    0.000391
Neutral Organics     : Green Algae   96-hr     ChV      0.00163 *
Neutral Organics     : Fish  (SW)    96-hr     LC50     0.00141 *
Neutral Organics     : Mysid Shrimp  96-hr     LC50   1.06e-006

                                                       mg/kg (ppm)
                                                        dry wt soil
                                                       ===========
Neutral Organics     : Earthworm     14-day    LC50       21.174 *

 Note:  * = asterick designates: Chemical may not be soluble
        enough to measure this predicted effect.
         Fish and daphnid acute toxicity log Kow cutoff: 5.0
         Green algal EC50 toxicity log Kow cutoff: 6.4
         Chronic toxicity log Kow cutoff: 8.0
         MW cutoff: 1000
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 23, 2003

Order number for sorting:

Remarks:

4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)

Test Substance

Identity:	Nitriles, C14-18 and C16-18, unsaturated (CAS RN 68513-04-2)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Green Algae
Analytical monitoring:	NA
Exposure period:	96-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	96-hour EC_{50} = not calculable
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CC=CC=CCCCC=CCCCCC
CHEM   : Nitriles, C14-18 and C16-18-unsatd.
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C16 H25 N1
MOL WT : 231.38
Log Kow: 6.08  (KowWin estimate)
Melt Pt:
Wat Sol: 0.07091 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Allylic/Vinyl Nitriles


                                                                  Predicted
ECOSAR Class              Organism    Duration  End Pt   mg/L (ppm)
========================  ==========  ========  ======   ==========
Neutral Organic SAR     : Fish        14-day    LC50        0.087 *
(Baseline Toxicity)

Allylic/Vinyl Nitriles  : Fish        96-hr     LC50        0.276 *

 Note:  * = asterick designates: Chemical may not be soluble
            enough to measure this predicted effect.
         Fish and daphnid acute toxicity log Kow cutoff: 5.0
         Green algal EC50 toxicity log Kow cutoff: 6.4
         Chronic toxicity log Kow cutoff: 8.0
         MW cutoff: 1000
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 23, 2003

Order number for sorting:

Remarks:

4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)

Test Substance

Identity:	Nitriles, C16 and C18 unsaturated (CAS RN 68002-64-2)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Green Algae
Analytical monitoring:	NA
Exposure period:	96-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	96-hour EC_{50} = 0.003 mg/l
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCCCCCCC=CCC=CCCCCC
CHEM   : Nitriles, C16 and C18-unsatd.
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C18 H31 N1
MOL WT : 261.45
Log Kow: 7.28  (KowWin estimate)
Melt Pt:
Wat Sol: 0.004784 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Neutral Organics


                                                                  Predicted
ECOSAR Class            Organism      Duration  End Pt  mg/L (ppm)
======================  ============  ========  ======  ==========
Neutral Organic SAR  : Fish          14-day    LC50       0.009 *
(Baseline Toxicity)

Neutral Organics     : Fish          96-hr     LC50       0.002
Neutral Organics     : Fish          14-day    LC50       0.009 *
Neutral Organics     : Daphnid       48-hr     LC50       0.003
Neutral Organics     : Green Algae   96-hr     EC50       0.003
Neutral Organics     : Fish          30-day    ChV     0.000636
Neutral Organics     : Daphnid       16-day    EC50     0.00168
Neutral Organics     : Green Algae   96-hr     ChV        0.006 *
Neutral Organics     : Fish  (SW)    96-hr     LC50       0.006 *
Neutral Organics     : Mysid Shrimp  96-hr     LC50     1.4e-005

                                                        mg/kg (ppm)
                                                        dry wt soil
                                                        ===========
Neutral Organics     : Earthworm     14-day    LC50       38.033 *

 Note:  * = asterick designates: Chemical may not be soluble
            enough to measure this predicted effect.
          Fish and daphnid acute toxicity log Kow cutoff: 5.0
          Green algal EC50 toxicity log Kow cutoff: 6.4
          Chronic toxicity log Kow cutoff: 8.0
          MW cutoff: 1000
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 23, 2003

Order number for sorting:

Remarks:

4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)

Test Substance

Identity:	9-Octadecenenitrile, (Z)- (CAS RN 112-91-4)
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Green Algae
Analytical monitoring:	NA
Exposure period:	96-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run using the following measured physical chemical properties: melting point = -1°C and boiling point = 330°C.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	96-hour EC_{50} = 0.0018 mg/l
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCCCCCCC=CCCCCCCCC
CHEM   : 9-Octadecenenitrile, (Z)-
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C18 H33 N1
MOL WT : 263.47
Log Kow: 7.50  (KowWin estimate)
Melt Pt: -1.00 deg C
Wat Sol: 0.006155 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Neutral Organics
```

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	0.006
Neutral Organics	: Fish	96-hr	LC50	0.00132
Neutral Organics	: Fish	14-day	LC50	0.006
Neutral Organics	: Daphnid	48-hr	LC50	0.002
Neutral Organics	: Green Algae	96-hr	EC50	0.00178
Neutral Organics	: Fish	30-day	ChV	0.000413
Neutral Organics	: Daphnid	16-day	EC50	0.00118
Neutral Organics	: Green Algae	96-hr	ChV	0.004
Neutral Organics	: Fish (SW)	96-hr	LC50	0.004
Neutral Organics	: Mysid Shrimp	96-hr	LC50	7.51e-006

				mg/kg (ppm) dry wt soil
Neutral Organics	: Earthworm	14-day	LC50	32.789 *

```
 Note:  * = asterick designates: Chemical may not be soluble
            enough to measure this predicted effect.
          Fish and daphnid acute toxicity log Kow cutoff: 5.0
          Green algal EC50 toxicity log Kow cutoff: 6.4
          Chronic toxicity log Kow cutoff: 8.0
          MW cutoff: 1000
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 23, 2003

Order number for sorting:

Remarks:

4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)

Test Substance

Identity:	Propionitrile, 3-(9-Octadecenylamino)- [CAS RN 26351-32-6; Propanenitrile, 3-(9-Octadecenylamino)-, (Z)-]
Purity:	NA

Method

Method/Guideline followed:	EPIWIN (v 3.10) ECOSAR Submodel (V 0.99g)
Type:	NA
GLP:	NA
Year:	2003
Species/Strain/Supplier:	Green Algae
Analytical monitoring:	NA
Exposure period:	96-hour
Statistical methods:	NA
Remarks:	The EPIWIN model was run without inputting physical chemical property values because measured values were not available.

Results

Nominal concentrations (mg/l):	NA
Measured concentrations (mg/l):	NA
Unit:	mg/l
Element value:	96-hour EC_{50} = not toxic at solubility
Statistical results:	NA
Remarks:	Following are the results from the model:

```
ECOSAR Program (v0.99g) Results:
================================
SMILES : C(#N)CCNCCCCCCCCC=CCCCCCCCC
CHEM   : Propionitrile, 3-(9-octadecenylamino)-
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C21 H40 N2
MOL WT : 320.57
Log Kow: 7.47  (KowWin estimate)
Melt Pt:
Wat Sol: 0.003754 mg/L  (calculated)
```

```
ECOSAR v0.99g Class(es) Found
-----------------------------
Aliphatic Amines
```

ECOSAR Class		Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	:	Fish	14-day	LC50	0.007 *
Aliphatic Amines	:	Fish	96-hr	LC50	0.028 *
Aliphatic Amines	:	Daphnid	48-hr	LC50	0.004 *
Aliphatic Amines	:	Green Algae	96-hr	EC50	0.052 *
Aliphatic Amines	:	Green Algae	96-hr	ChV	0.041 *

```
 Note:  * = asterick designates: Chemical may not be soluble
            enough to measure this predicted effect.
          Fish and daphnid acute toxicity log Kow cutoff: none
          Green algal EC50 toxicity log Kow cutoff: none
          Chronic toxicity log Kow cutoff: none
          MW cutoff: none
```

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group)

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions; model data.

References

US EPA. 2000. ECOSAR Program, Risk Assessment Division (7403). US Environmental Protection Agency, Washington, DC.

Other

Last changed: May 26, 2003

Order number for sorting:

Remarks:

4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)

Test Substance

Identity:	Tallow nitrile (CAS RN 61790-28-1; Nitriles, tallow)
Purity:	Purity provided as percent distribution of Carbon chain length from C_{12} to C_{20}.
Remarks:	

Method

Method/Guideline followed:	OECD Guideline 201 "Algae, Growth Inhibition Test"
Test type:	Not stated
GLP:	Yes
Year:	1992
Species/Strain/Supplier:	*Scenedesmus subspicatus* CHODAT/Algensammlung, Göttingen, SAG 86.81
Element basis:	Biomass and growth rate
Exposure period:	72 hours
Analytical monitoring:	No
Statistical methods:	EC-Regulation from Tallarida, R. J. Jacob, L. S. (1979): The dose-response relation in pharmacology. 98-103, Springer-Verlag; and Bestimmung der Biomasse-Hemmung und der ratenbezogenen Hemmung gem. DIN 38412 L9 analog OECD-Guideline 201
Remarks:	Ultrasonic dispersion at 40°C with Tween 80

Results

Nominal concentrations (mg/l):	0.1, 0.32, 1.0, 3.2, 10.0 mg/l
Measured concentrations (mg/l):	Not stated
Unit:	mg/l
Element value:	72-hour EC_{50}
Result:	72-hour EC_{50} for biomass = 0.497 mg/l 72-hour EC_{50} for growth rate = 0.619 mg/l
Satisfactory control response:	Not stated
Statistical results:	Not stated
Remarks:	NOEC for biomass < 0.10 mg/l NOEC for growth rate = 0.32 mg/l

Conclusions

Remarks:	The 72-hour growth inhibition has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study (OECD).

References

Noack, U. 1992. Study of algal growth inhibition by tallow nitrile. Test number SSO27472. Dr. U. Noack Laboratories for Applied Biology, Hildesheim, Germany.

Other Available Reports

IUCLID (update 23-Oct-95).
Hoechst: Unpublished document (Noack SSO27472, 10.07.1992)

Other

Last changed:	April 17, 2001
Order number for sorting:	33-37
Remarks:	

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Dodecanenitrile (CAS RN 2437-25-4)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	OECD Guideline 401 "Acute Oral Toxicity"
Type:	LD_{50}
GLP:	Yes
Year:	1987
Species/Strain:	Rat (Strain not stated)
Sex:	Not stated
No. of animals per sex per dose:	Not stated
Vehicle:	Not stated
Route of administration:	Not stated
Remarks:	

Results

Value:	LD_{50} > 2.0 g/kg
Number of deaths:	Not stated
Remarks:	

Conclusions

Remarks:	The acute oral LD_{50} has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restriction; IUCLID summary of study conducted to guideline.

References Hoechst. 1987. Unpublished document (87.1674). Cited in IUCLID (update 23-Oct-95).

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	5
Remarks:	

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Laurylnitrile (CAS RN 2437-25-4; Dodecanenitrile)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	OECD Guideline 401 "Acute Oral Toxicity"
Type:	LD_{50}
GLP:	Yes
Year:	1987
Species/Strain:	Rat (Strain not stated)
Sex:	Not stated
No. of animals per sex per dose:	Not stated
Vehicle:	Not stated
Route of administration:	Not stated
Remarks:	

Results

Value:	LD_{50} 3.4 g/kg
Number of deaths:	Not stated
Remarks:	

Conclusions

Remarks:	The acute oral LD_{50} has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restriction; IUCLID summary of study conducted to guideline.

Reference Oleofina. S.C.K. – C.E.N. Study: AO87102 (B-2400 Mol, Belgium). Cited in IUCLID (update 23-Oct-95).

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	5c
Remarks:	

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Arneel OD (CAS RN 112-91-4, 9-Octadecenenitrile)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	FIFRA (40 CFR)
Type:	LD_{50} limit test
GLP:	Yes
Year:	1987
Species/Strain:	Sprague-Dawley rat
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	None
Route of administration:	Oral gavage
Remarks:	Five male and five female young adult Sprague-Dawley rats weighing between 154 and 244 g were dosed orally with the test substance at 5.0 g/kg. Animals were fasted overnight prior to dosing. All animals were fitted with collars following dosing for the duration of the test to prevent the spread of test material when preening. Animals were observed 1, 2 and 4 hours post dose and once each morning and afternoon thereafter for 14 days for mortality, toxicity and pharmacological effects. Body weights were recorded immediately pretest, weekly and at termination. All animals were killed by CO_2 inhalation, dipped ten times in isopropanol, (in an attempt to collect the "oily" residue on the body surface) and given a gross necropsy. The isopropanol was evaporated and the residue sent to the sponsor.

Results

Value:	LD_{50} > 5.0 g/kg
Number of deaths:	0
Remarks:	All animals survived the 14-day observation period. Clinical signs associated with the test material were piloerectoin, urine stains, scruffy hair coat, red-brown stains around the nose, coats oily on the dorsal side, alopecia on the back (one female, two males) and alopecia on the hind legs (two females, three males). All animals gained weight throughout the observation period. Necropsy results were

normal in nine of the ten animals. The left kidney of one female appeared slightly hollowed.

Conclusions

Remarks: The acute oral LD_{50} has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch): 1A
Remarks: Reliable without restriction; guideline study.

References

Doyle, R. L. Acute oral toxicity limit test in male and female rats. 1987. Project number 87-0323-21. Hill Top Biolabs, Inc., Miamiville, OH, U. S.

Other Available Reports

Other

Last changed: January 5, 2004
Order number for sorting: 2a
Remarks:

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	(CAS RN 61789-53-5; Nitriles, coco)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	OECD Guideline 401 "Acute Oral Toxicity"
Type:	LD_{50}
GLP:	Yes
Year:	1985
Species/Strain:	Rat (Strain not stated)
Sex:	Not stated
No. of animals per sex per dose:	Not stated
Vehicle:	Not stated
Route of administration:	Not stated
Remarks:	

Results

Value:	LD_{50} > 2.0 g/kg
Number of deaths:	Not stated
Remarks:	

Conclusions

Remarks:	The acute oral LD_{50} has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restriction; IUCLID summary of study conducted to guideline.

References KENOGARD. 1985. Huntingdon Research Center report number 85298D/KND 4/AC. Cited in IUCLID (update 23-Oct-95).

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	20
Remarks:	

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	FARNIL TH-D (CAS RN 61790-29-2; Nitriles, tallow, hydrogenated)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	Directive of the Commission of European Communities 92/69/CEE Annex, Part B, Method B. 1 bis.
Type:	Fixed dose method
GLP:	Yes
Year:	1995
Species/Strain:	Rat/Wistar Crl:(WI)BR
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	Tween 80 at 5% in bidistilled water
Route of administration:	Oral gastric intubation
Remarks:	A group of ten rats (five males and five females), weighing 118 to 132 g and approximately five weeks old at test initiation, were administered the test substance suspended in Tween 80 as 5% in bidistilled water orally by gastric intubation at a concentration of 2000 mg/kg. A single dose was given at a volume of 10 ml/kg. Rats were observed frequently on the day of test substance administration and at least twice daily for 14 days. At the end of the 14-day observation period, rats were sacrificed and subjected to a necropsy.

Results

Value:	Not determined
Number of deaths:	0/10
Remarks:	All rats survived until study termination. Clinical observations noted in all rats during the first two days post dose included hunched back and piloerection. During the remainder of the observation period, no alterations were observed in any of the rats. All rats gained weight during the 14-day observation period. No visible treatment-related macroscopic lesions were noted during necropsy in any rat.

Conclusions

Remarks:	According to the results obtained and the classification set out by the Directive of the Commission of European Communities 92/69/CEE Annex, Part B, Method B. 1 bis.,

it can be concluded that the substance FARNIL TH-D is free of any significant toxicity. (Author of report)
The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch): 1C
Remarks: Reliable without restriction; test procedure according to national standards.

References

Tortajada, J. 1995. Acute oral toxicity test in rats. fixed dose method. Report number CD-95/4287T. Centro de Investigación y desarrollo Aplicado, S.A.L., Barcelona, Spain.

Other

Last changed: April 17, 2001
Order number for sorting: 4d
Remarks:

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Tallow-nitrile (CAS RN 61790-28-1; Nitriles, tallow)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	OECD Guideline 401 "Acute Oral Toxicity"
Type:	LD_{50}
GLP:	Yes
Year:	1987
Species/Strain:	Rat (Strain not stated)
Sex:	Not stated
No. of animals per sex per dose:	Not stated
Vehicle:	Not stated
Route of administration:	Not stated
Remarks:	

Results

Value:	LD_{50} > 6.0 g/kg
Number of deaths:	Not stated
Remarks:	

Conclusions

Remarks:	The acute oral LD_{50} has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restriction; IUCLID summary of study conducted to guideline.

References FINA Chemicals. SCK-CEN (B-2400 Mol, Belgium) Study AO87103. Cited in IUCLID (update 23-Oct-95).

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	37 - I15
Remarks:	

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Tallow-nitrile (CAS RN 61790-28-1; Nitriles, tallow)
Purity:	Purity provided as percent distribution of carbon chain length from C12 to C20.
Remarks:	

Method

Method/guideline followed:	OECD Guideline 401 "Acute Oral Toxicity"
Type:	LD_{50}
GLP:	Yes
Year:	1987
Species/Strain:	Rat (Strain not stated)
Sex:	Not stated
No. of animals per sex per dose:	Not stated
Vehicle:	Not stated
Route of administration:	Not stated
Remarks:	

Results

Value:	LD_{50} > 2.0 g/kg
Number of deaths:	Not stated
Remarks:	

Conclusions

Remarks:	The acute oral LD_{50} has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	1D
Remarks:	Reliable without restriction; guideline with minimal data provided.

References

Jung, A. 1987. Short report: acute toxicity per OS. Report number 87.1717. PHARMA Research Toxicology.

Other Available Reports

Hoechst. 1987. Unpublished document (87-1717). Cited in IUCLID (update 23-Oct-95).

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	35-37

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Arneel TMD (CAS RN 61790-28-1; Nitriles, tallow)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	EPA Health Effects Guidelines
Type:	LD_{50} limit test
GLP:	Yes
Year:	1986
Species/Strain:	Wistar rat
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	None
Route of administration:	Oral gavage
Remarks:	Five male and five female Wistar albino rats approximately 8 weeks old and weighing between 238 and 298 g were dosed orally with the test substance at 5.0 g/kg. Animals were fasted for 16-20 hours prior to dosing. Animals were observed 1, 2 and 4 hours post dose and once each morning and afternoon thereafter for 14 days for mortality, toxicity and pharmacological effects. Body weights were recorded immediately pretest, weekly and at termination. All animals were examined for gross pathology. Abnormal tissues were preserved in 10% neutral buffered formalin for possible future microscopic examination.

Results

Value:	$LD_{50} > 5.0$ g/kg
Number of deaths:	0
Remarks:	All animals survived the 14-day observation period. Oily appearance of body surface was during study days 1 through 3 . One animal had respiratory rales on Day 6. All animal appeared normal from Day 7 through Day 14. All but one animal gained weight throughout the observation period. Necropsy results were normal in eight of the ten animals. Abnormalities of the intestine were noted in one animal and an abnormality of the left ovary in another animal.

Conclusions

Remarks:	The acute oral LD_{50} has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Cerven, D. R. Single dose oral toxicity in rats/LD_{50} in rats. 1986. Project number MB 85-8045 A. MB Research Laboratories, Inc., Spinnerstown, PA, U. S.

Other Available Reports

Other

Last changed:	January 5, 2004
Order number for sorting:	38
Remarks:	

5.5 GENETIC TOXICITY *IN VITRO*

Test Substance

Identity:	Dodecanenitrile (CAS RN 2437-25-4)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	OECD guideline 471 and 472
Type:	Reverse mutation assay
System of testing:	Bacterial
GLP:	Yes
Year:	1988
Species/Strain:	*Salmonella typhimurium* TA98, TA100, TA1535, TA 1537 and TA1538, and *Escherichia coli* WP2uvrA
Metabolic activation:	With and without activation
Concentrations tested:	Not stated
Statistical methods:	Not stated
Remarks:	

Results

Result:	Negative
Cytotoxic concentration:	Not stated
Genotoxic effects:	Not stated
Statistical results:	Not stated
Remarks:	

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restriction; IUCLID summary of study conducted to guideline.

References Hoechst. 1988. Unpublished document (88.1477). Cited in IUCLID (update 23-Oct-95).

Other Available Reports

Other

Last Changed:	January 5, 2004
Order Number for Sorting:	5
Remarks:	

5.5 GENETIC TOXICITY *IN VITRO*

Test Substance

Identity:	Talgnitril (CAS RN 61790-28-1; Nitriles, tallow)
Purity:	Approximately 99%
Remarks:	

Method

Method/guideline followed:	OECD Method No. 471, *Salmonella typhimurium*, Reverse Mutation Test; OECD Method No. 472, *Escherichia coli*, Reverse Mutation Assay
Type:	Reverse mutation assay
System of testing:	Bacterial
GLP:	Yes
Year:	1988
Species/Strain:	*Salmonella typhimurium* strains TA 1535, TA 1537, TA 1538, TA 98 and TA 100; *Escherichia coli* strain WP2uvrA
Metabolic activation:	With and without S-9 activation; S-9 mix obtained from the liver of Arochlor 1254-induced male Sprague Dawley rats; S-9 mix was prepared at the laboratory; 0.5 ml/plate was used
Concentrations tested:	10,000, 5000, 2500, 500, 100, 20, 4 and 0 µg/plate
Statistical methods:	None
Remarks:	Two independent experiments were conducted and three replicates per dose were tested in each experiment. Plates were dosed once. In both experiments, the test substance was dissolved in the solvent DMSO. In the first experiment, the test substance was tested for signs of toxicity at doses of 4 to 10,000 µg/plate. In the second experiment, which tested mutagenicity of the test substance, 5000 µg/plate was chosen as the highest dose. The mutagenicity study was conducted in the absence and in the presence of metabolic activation. Positive control plates were included for each strain. The following substances were used as positive controls without metabolic activation: Na-azide (TA100 and TA1535), 9-aminoacridine (TA1537), 2-nitrofluorene (TA98 and TA1538) and n-methyl-n-nitro-n-nitrosoguanidine (WP2uvrA). The following substances were used as positive controls with metabolic activation: benzo[a]pyrene (TA98, TA100, TA1535, TA1537, TA1538 and WP2uvrA) and 2-aminoanthracene (TA98, TA100, TA1535, TA1537, TA1538 and WP2uvrA).

Results

Result:	The test substance was not mutagenic in the bacterial test system either in the absence or in the presence of metabolic activation under the conditions of this test.
Cytotoxic concentration:	None
Genotoxic effects:	Negative
Statistical results:	None
Remarks:	The test substance proved to be not toxic to the bacterial strains tested up to 10,000 µg/plate. Visible precipitation of the test substance on the plates was observed at concentrations of 500 µg/plate and higher. The test substance did not cause a significant increase in the number of revertant colonies with any of the tester strains either in the absence or presence of metabolic activation at dose levels ≤ 5000 µg/plate. No dose-dependent effect was observed.

Conclusions

Remarks:	When tested at dose levels up to 5000 µg/plate in DMSO, talgnitril was not mutagenic in this bacterial test system. (Author of report) The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Nitriles Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Müller, W. 1988. Study of the mutagenic potential in strains of *Salmonella typhimurim* (Ames Test). Report number 88.1690. Pharma Research Toxicology and Pathology, Frankfurt, Germany.

Other Available Reports

Other

Last changed:	April 17, 2001
Order number for sorting:	36
Remarks:	